National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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Aitken Rome Nodes Upgraded from TOSS3 to TOSS4

- Systems experts completed the transition of the default operating system for AMD Rome nodes of the Aitken supercomputer from Red Hat Enterprise Linux Tri-lab Operating System Stack (TOSS3) (RHEL 7) to TOSS4 (RHEL 8).
- TOSS4 is compliant with the most up-to-date agency security requirements and is optimized for efficiently running large-scale HPC workloads.
- HECC is leveraging interagency HPC work in operating systems and application scaling. Each organization will be contributing improvements to the TOSS kernel.
- The Aitken supercomputer consists of 2,048 AMD Rome compute nodes and 1,152 Intel Cascade Lake compute nodes. The system represents HECC's cutting-edge supercomputing capability and ranked #63 on the November 2022 TOP500 list with a sustained rate of 9.07 petaflops on the linear equations software package (LINPACK) benchmark.
- One of the major efforts in transitioning to TOSS4 was to work with the user community to identify and remediate software compatibility and workflow issues to ensure that the migration had minimal impact on our userbase.
- The biggest challenge of the migration from TOSS3 to TOSS4 was performing the upgrade while training additional staff on system processes and the Rome architecture.

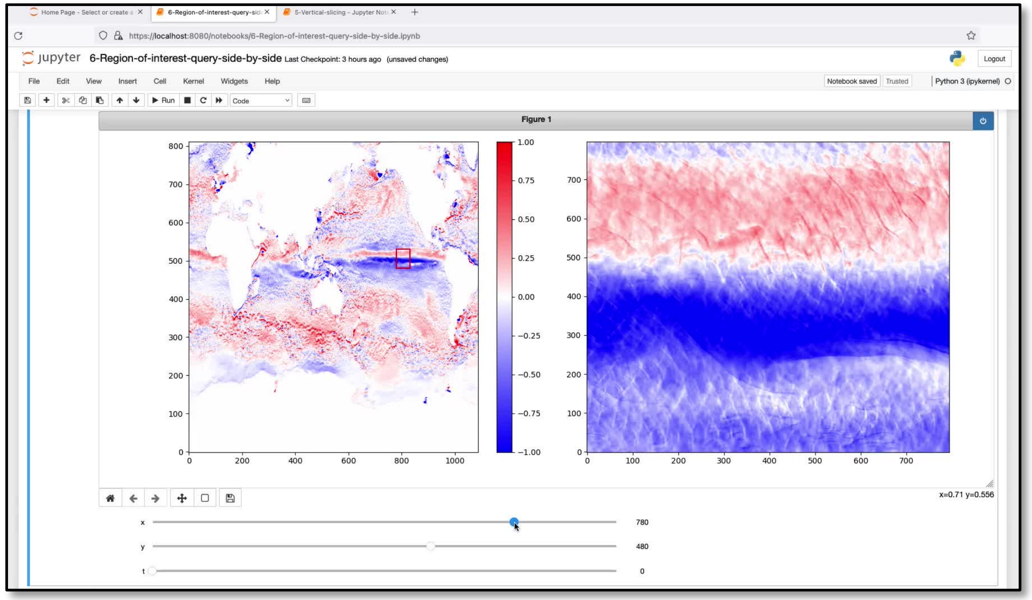
IMPACT: Upgrading to TOSS4 ensures compliance with a NASA mandate that sunsets RHEL 7-based operating systems. TOSS3 is built on RHEL 7 and contains Python 2.7, which was phased out due to security concerns.

The Tri-Lab Operating System Stack (TOSS) emblem, *credit to Lawrence Livermore National Laboratory*

Visualization Experts Support a Flexible Encoding Framework for Streaming Large Scientific Datasets

- HECC's Visualization and Data Analysis team is providing guidance and technical assistance to researchers from the University of Utah's Scientific Computing and Imaging (SCI) Institute, who are leveraging their latest research in extreme-scale data management, analysis, and visualization to support progressive streaming of large scientific data.
- In year 1 of a two-year collaborative agreement, the HECC team collaborated with SCI researchers and climate scientists to apply the framework to the GEOS-MITgcm coupled atmosphere-ocean simulation output, and to explore the use of Jupyter Notebooks as a mechanism for remote streaming and interactive visualization of encoded data stored on the Pleiades supercomputer.
  - The flexible encoding framework, in-memory data structure supports progressive decompression in both resolution and precision, as well as fast data access and querying through the use of block partitioning and caching.
  - The anticipated novel runtime system will automate data reduction and resource allocation decisions for in-situ workflows, adaptively satisfying a range of user, application, and system constraints.
- In year 2, the Visualization team will continue assisting researchers as they further improve their framework, develop and integrate the autonomic runtime system, apply the work to additional datasets, and further explore mechanisms for remote streaming and visualization.

IMPACT: Optimizing data management, analysis, and visualization workflows can help HECC users achieve their scientific goals more quickly and/or with fewer resources.



Screen recording of an interactive session with two proof-of-concept Jupyter Notebooks (shown at 4x playback speed) featuring MITgcm east-west ocean velocity data. The notebooks support interactively selecting and animating regions of interest and exploring vertical cross-sections across time.

HECC Staff Return to In-Person NASA Exhibit at SC22

- HECC staff planned and produced NASA's booth at SC22, the International Conference for High-Performance Computing, Networking, Storage, and Analysis, held November 13-18 in Dallas, TX, interfacing with more than 11,000 attendees in the Agency's first in-person return to the annual conference since 2019.
- 36 in-person and virtual presentations by scientists and researchers from four NASA centers, as well as university and industry collaborators, showcased projects enabled by NASA High-End Computing resources and services provided by the High-End Computing Capability project and the NASA Center for Climate Simulation.
- Working with agency and vendor partners, a wide array of high-resolution images and videos of science and engineering simulations, many created by HECC visualization experts, were shown on the booth's nine-panel hyperwall, and were made available to virtual attendees on the NASA@SC22 website along with written abstracts for each presentation.

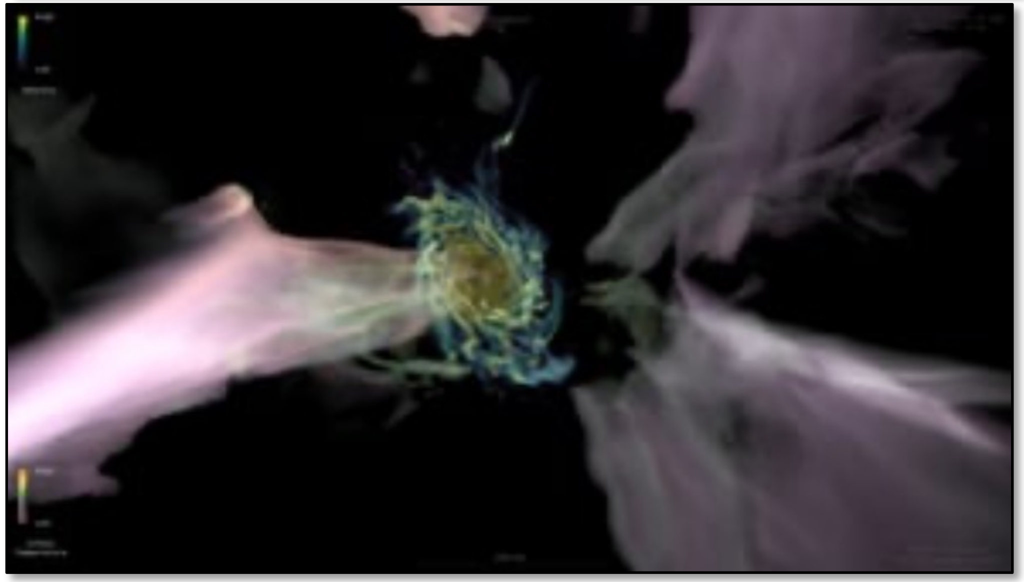
IMPACT: The annual Supercomputing Conference provides a highly visible public platform to showcase NASA science and engineering missions supported by the agency's high-performance computing resources, as well as NASA's latest research and advances in computing technologies.

The SC22 exhibit support team and presenters representing all mission directorates provided thousands of conference attendees with a memorable NASA experience.

Pleiades Simulations Track the Fuel for Galaxy Growth*

- As part of the Figuring Out Gas & Galaxies in Enzo (FOGGIE) project, astrophysicists from the Space Telescope Science Institute and Johns Hopkins University ran high-resolution cosmological hydrodynamic simulations on Pleiades to investigate the diffuse gas surrounding galaxies, the circumgalactic medium (CGM).
- By resolving the small-scale interactions between inflowing gas, outflowing gas, and gas at a variety of temperatures and densities, the FOGGIE simulations indicated that most of the CGM gas accreting onto galaxies is cooler than the rest of the CGM gas that is not flowing inward, and hasn't been affected by the heavy elements that are formed in stars, suggesting that it is nearly pristine gas that has never been located near another galaxy.
- The simulations are helping the researchers gain understanding of how this fresh gas reaches a galaxy and what happens to it along the way through the CGM. Since galaxies form new stars out of gaseous material that is accreted from the CGM, understanding the properties and origin of this material is fundamental to understanding galaxy evolution.
- HECC resources are necessary to simulate the nearly 200 million resolution elements in the gas and stars in and around the galaxies; store the resulting hundreds of terabytes of output files; and produce and analyze the visualizations made possible by HECC's visualization team.

IMPACT: These high-resolution, realistic simulations of galaxies help interpret data from observations made by NASA's Hubble and James Webb Space Telescopes, and make predictions for the difficult-to-observe parts of galaxies. The project addresses NASA's strategic goal to understand the universe.



Visualization of a FOGGIE simulation in which many galaxies merge over time to make one galaxy. Gas density is shown in blue-green-yellow; inflowing gas is highlighted in a purple-green according to temperature. *Cassi Lochhaas, Space Telescope Science Institute; Chris Henze, NASA/Ames*

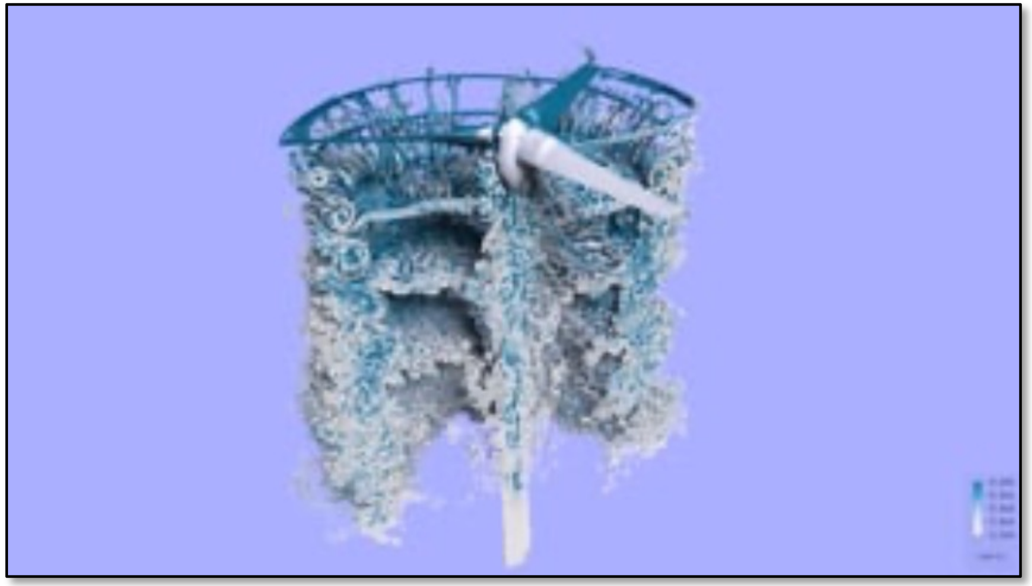
** HECC provided supercomputing resources and services in support of this work.*

A Decade of Discovery in Rotorcraft Simulation*

- Over the last 10 years, NASA Ames researchers have run simulations at the NASA Advanced Supercomputing (NAS) facility to improve the accuracy of rotorcraft hover performance by 10x.
  - In 2009, computational fluid dynamics (CFD) prediction accuracy for rotorcraft hover performance differed from experiment by 2.4%—a significant discrepancy for rotorcraft operations.
- Through NASA's Revolutionary Vertical Lift Technology (RVLT) Project, the researchers worked to understand this shortcoming. Their advanced techniques, such as algorithm improvements and adaptive mesh refinement, reduced the CFD error for rotorcraft from 2.4% to 0.2%—an order-of-magnitude improvement at a quarter of the computational cost.
- The CFD advances led to the discovery of turbulent worms—a previously unknown phenomenon found in the rotor wake. And, for the first time, simulations showed that blade-vortex interaction (BVI) can cause dynamic stall on the UH60 Blackhawk helicopter.
- Time-dependent flow animations created by NAS visualization experts played a crucial role in connecting cause and effect to understand the physics of rotorcraft flows.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Improvements in computational fluid dynamics simulation methods lead to new understanding of how numerical choices affect the physics of rotorcraft hover and forward flight—demonstrating the power of discovery made through NASA high-end computing resources.



This time-dependent animation shows the interior flow physics of the rotor wake for a V22 Osprey rotor in hover. Unprecedented detail revealed a new flow phenomenon, small spinning structures called turbulent worms. *Neal M. Chaderjian, Timothy Sandstrom, NASA/Ames*

Papers

- “**Confirmation and Characterisation of Three Giant Planets Detected by TESS from the FIES/NOT and Tull/McDonald Spectrographs**,” E. Knudstrup, et al., Astronomy & Astrophysics, vol. 667, November 3, 2022. *
  https://www.aanda.org/articles/aa/abs/2022/11/aa43656-22/aa43656-22.html
- “**Multi-Fluid Simulations of Upper Chromospheric Magnetic Reconnection with Helium-Hydrogen Mixture**,” Q. Wargnier, et al., arXiv:2211.02157 [astro-ph.SR], November 3, 2022. *
  https://arxiv.org/abs/2211.02157
- “**Predicting Char Yield of High-Temperature Resins**,” J. Gissinger, et al., Carbon, vol. 202, pt. 1, November 4, 2022. *
  https://www.sciencedirect.com/science/article/abs/pii/S0008622322009150
- “**An Improved MHD Simulation of the 2006 December 13 Coronal Mass Ejection of Active Region NOAA 10930**,” Y. Fan, arXiv:2211.03736 [astro-ph.SR], November 7, 2022. *
  https://arxiv.org/abs/2211.03736
- “**Multi-Fluid Simulation of Solar Chromospheric Turbulence and Heating Due to the Thermal Farley-Buneman Instability,**” S. Evans, et al., arXiv:2211.03644 [astro-ph.SR], November 7, 2022. *
  https://arxiv.org/abs/2211.03644
- “**Examining the Orbital Decay Targets KELT-9 b, KELT-16 b and WASP-4 b, and the Transit-Timing Variations of HD 97658 b**,” J.-V. Harre, et al., arXiv:2211.05646 [astro-ph.EP], November 10, 2022. *
  https://arxiv.org/abs/2211.05646

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Solar Flare Ribbon Fronts I: Constraining Flare Energy Deposition with IRIS Spectroscopy**," V. Polito, et al., arXiv:2211.05333 [astro-ph.SR], November 10, 2022. *
https://arxiv.org/abs/2211.05333
- "**TOI-1695 b: A Keystone Water World Elucidating Radius Valley Emergence Mechanisms Around Early M Dwarfs**," C. Cherubim, et al., arXiv:2211.06445 [astro-ph.EP], November 11, 2022. *
https://arxiv.org/abs/2211.06445
- "**Dispersal and Costal Geomorphology Limit Potential for Mangrove Range Expansion Under Climate Change**," J. Raw, et al., Journal of Ecology, published online November 13, 2022. *
https://besjournals.onlinelibrary.wiley.com/doi/full/10.1111/1365-2745.14020
- "**Strain-Induced Superfluid Transition for Atoms on Graphene**," S.-W. Kim, et al., arXiv:2211.07672 [cond-mat.mes-hall], November 14, 2022. *
https://arxiv.org/abs/2211.07672
- "**Tripolar Guide Magnetic Fields Due to Island Coalescence in Solar Wind Current Sheets: Simulation and Theory**," D. Newman, et al., Physics of Plasmas, vol. 29, issue 11, November 14, 2022. *
https://aip.scitation.org/doi/abs/10.1063/5.0102906

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- “**Computational Study of Boundary Layer Effects on Stochastic Rotor Blade Vortex Shedding Noise**,” C. Thurman, Aerospace Science and Technology, vol. 131, pt. A, November 15, 2022. *
https://www.sciencedirect.com/science/article/abs/pii/S1270963822006575
- “**The Impact of Multi-Fluid Effects in the Solar Chromosphere on the Ponderomotive Force under LTE and NEQ Ionization Conditions**,” J. Martinez-Sykora, et al., arXiv:2211.09361 [astro-ph.SR], November 17, 2022. *
https://arxiv.org/abs/2211.09361
- “**Efficient Quasi-Classical Trajectory Calculations by Means of Neural Operator Architectures**,” M. Sharma Priyadarshini, et al., Earth, Space, and Environmental Chemistry, published online November 17, 2022. *
https://chemrxiv.org/engage/chemrxiv/article-details/63751109082129f04af9b617
- “**As a Matter of Dynamical Range – Scale Dependent Energy Dynamics in MHD Turbulence**,” P. Grete, et al., arXiv:2211.09750 [astro-ph.GA], November 17, 2022. *
https://arxiv.org/abs/2211.09750
- “**Correction and Calibration of Atmospheric Impact Observations in GOES GLM Data**,” R. Morris, et al., Meteoritics & Planetary Science, published online November 24, 2022. *
https://onlinelibrary.wiley.com/doi/full/10.1111/maps.13926

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Presentations

- **Supercomputing 2022 (SC22)**, Dallas, Texas, November 13-18, 2022.
  - “**Computing at the Edge: A Discussion about Supporting Recent US Space Missions**,” D. Duffy, W. Thigpen, C. Batton, M. Fernandez, J. Ott.
    https://sc22.supercomputing.org/presentation/?id=pan118&sess=sess184
  - “**Wall-Modeled Large Eddy Simulations for Aircraft Certification-by-Analysis**,” C. Kiris.
    https://www.nas.nasa.gov/SC22/research/project1.html
  - “**NASA’s SUSAN Electrofan Aircraft: Designing the Future of Green Aviation**,” L. Machado.
    https://www.nas.nasa.gov/SC22/research/project2.html
  - “**Scale Resolving Jet Noise Simulations to Reduce Airport Noise**,” G.-D. Stich.
    https://www.nas.nasa.gov/SC22/research/project3.html
  - “**Predicting Buffet Onset on the Transonic Truss-Braced Wing**,” O. Browne.
    https://www.nas.nasa.gov/SC22/research/project4.html
  - “**A Decade of Discovery in Rotorcraft Simulation with NASA Supercomputing**,” N. Chaderjian.
    https://www.nas.nasa.gov/SC22/research/project5.html
  - “**Simulations for Designing Safe and Efficient Air Taxis**,” P. Ventura Diaz.
    https://www.nas.nasa.gov/SC22/research/project6.html
  - “**Advancing NASA Software for Sonic Boom Prediction**,” J. Duensing.
    https://www.nas.nasa.gov/SC22/research/project7.html
  - “**Multiphase Simulations of the Launch Environment at NASA’s Kennedy Space Center**,” J. Angel.
    https://www.nas.nasa.gov/SC22/research/project8.html

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Presentations

- **Supercomputing 2022** (cont).
  - "**Building Aerodynamic Databases for NASA's Space Launch System**," J. Meeroff. *https://www.nas.nasa.gov/SC22/research/project9.html*
  - "**Simulating Supersonic Parachute Inflation for Mars Landers**," C. Kiris, J. Angel. *https://www.nas.nasa.gov/SC22/research/project10.html*
  - "**HECC: Evolving to Meet Tomorrow's Requirements**," W. Thigpen. *https://www.nas.nasa.gov/SC22/research/project23.html*

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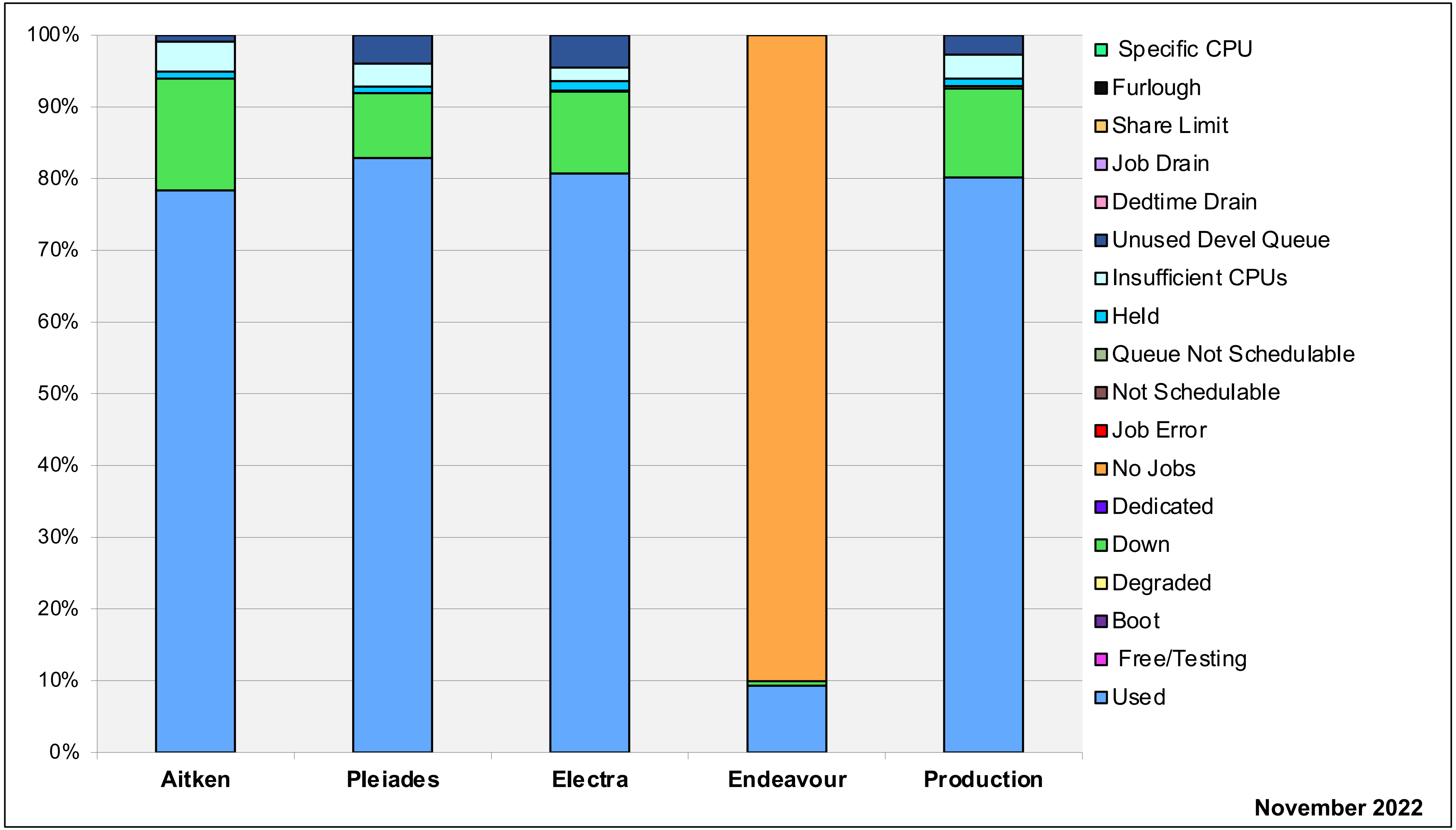
News and Events

- **2022 Road Trip: NASA Ames Takes Off**, *HPCwire*, November 25, 2022—In this interview with HPCwire contributing editor Dan Olds, NAS Division Chief Piyush Mehrotra talks all things supercomputing—from global ocean simulations to modular facilities, cloud applications, and new high-end computing system architectures at NASA's Ames Research Center.
https://www.hpcwire.com/2022/11/25/2022-road-trip-nasa-ames-takes-off/
- **5 Ways Supercomputing is Key to NASA Mission Success**, *NASA Ames*, November 22, 2022--Whether developing new technologies for landing on other planets improving air travel here at home with new air taxi concepts, or more realistically simulation global weather and climate on Earth and other planets—both inside and outside our solar system—supercomputing is the key to the success of NASA missions.
https://www.nasa.gov/feature/5-ways-supercomputing-is-key-to-nasa-mission-success
- **Secrets of Sunspots and Solar Magnetic Fields**, *NASA Ames*, November 17, 2022—Using data about the Sun's structure and dynamics from two NASA missions, the Solar and Heliospheric Observatory and the Solar Dynamics Observatory, researchers are running simulations on supercomputers at the NASA Advanced Supercomputing facility to learn more about the sunspot cycle.
https://www.nasa.gov/feature/ames/sunspot-simulations

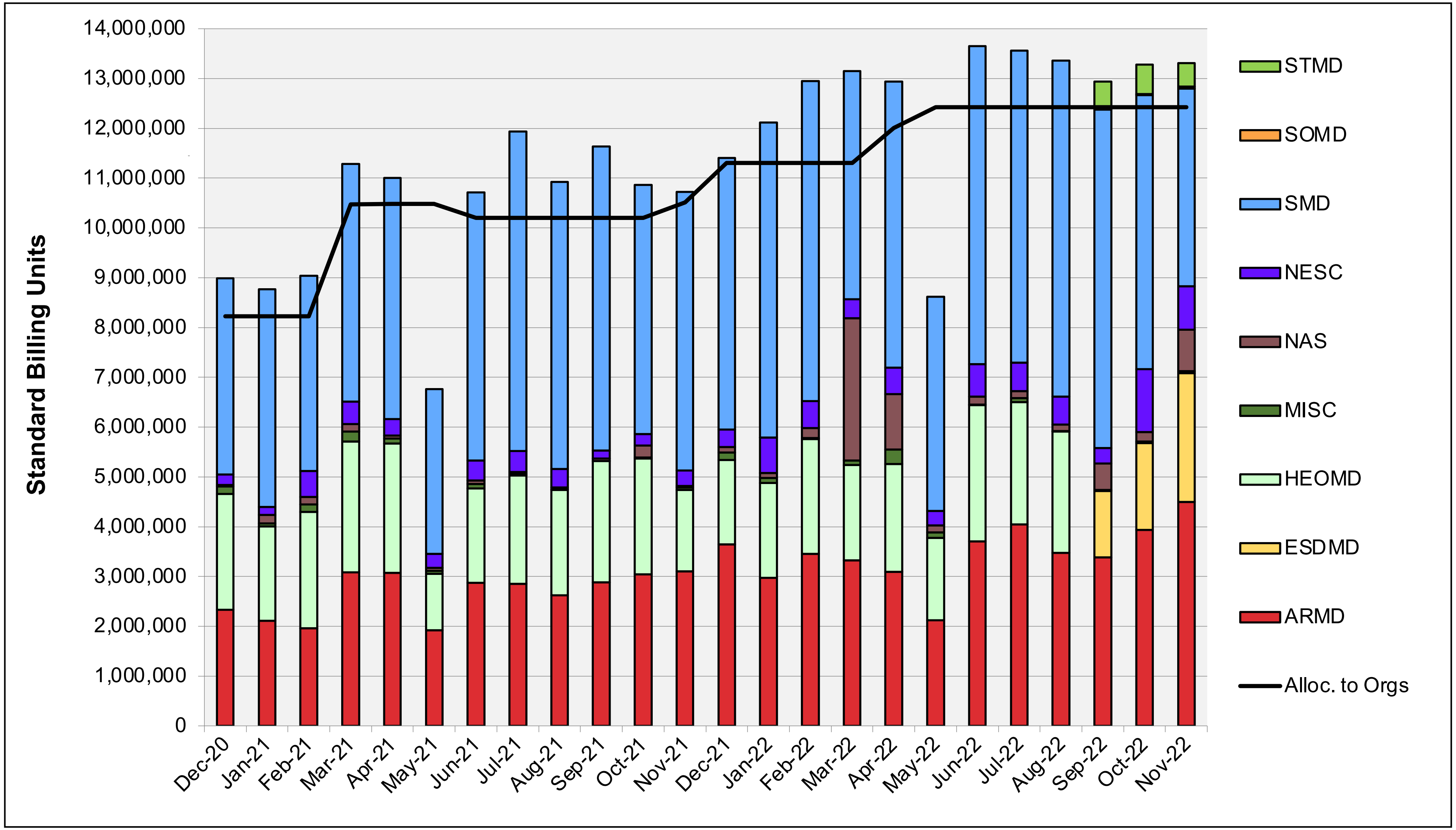
News and Events: Social Media

- **Coverage of NAS Stories**
  - NASA@SC22:
    - NASA Supercomputing: Twitter Collection
  - Ames Feature: Solar Magnetic Fields:
    - NASA Ames: Twitter 52 retweets, 163 likes; Facebook, 76 likes, 1.3K views.
  - Ames Feature: 5 Ways Supercomputer Support NASA Missions:
    - NASA Ames: Twitter 20 retweets, 80 likes; Facebook, 118 likes, 34 shares.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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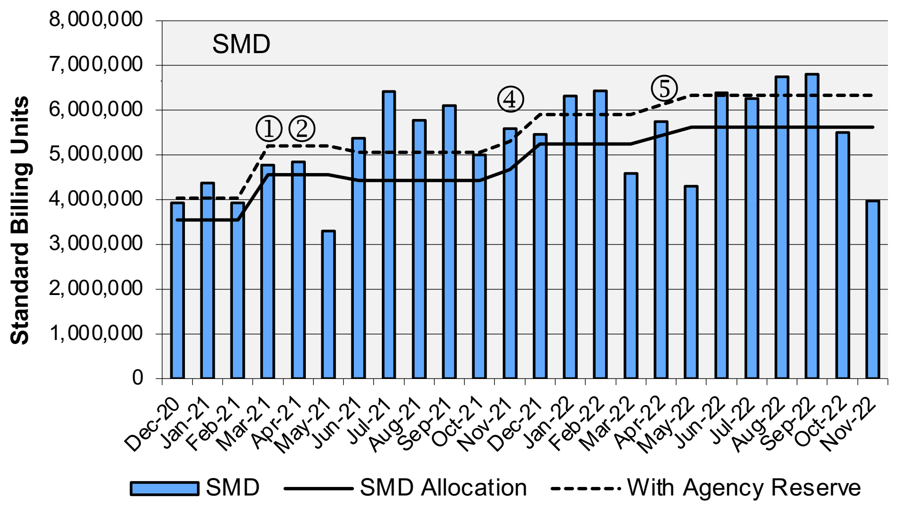
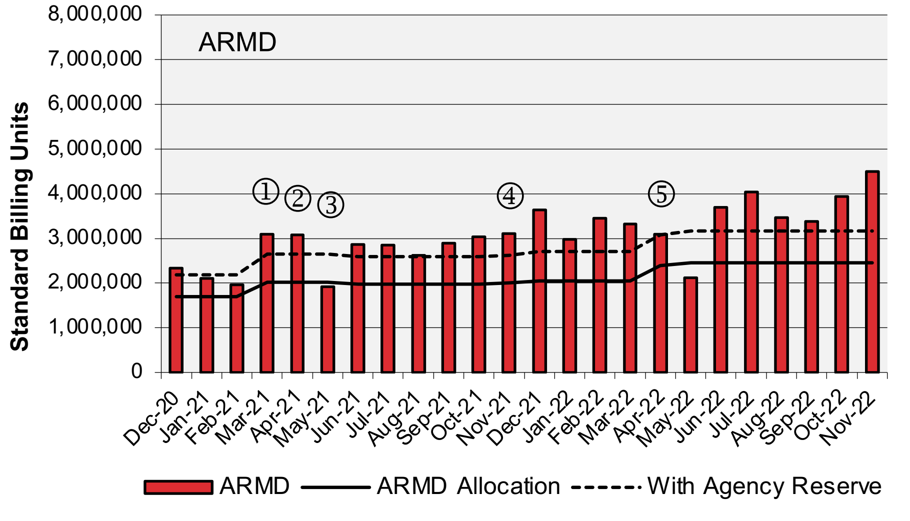
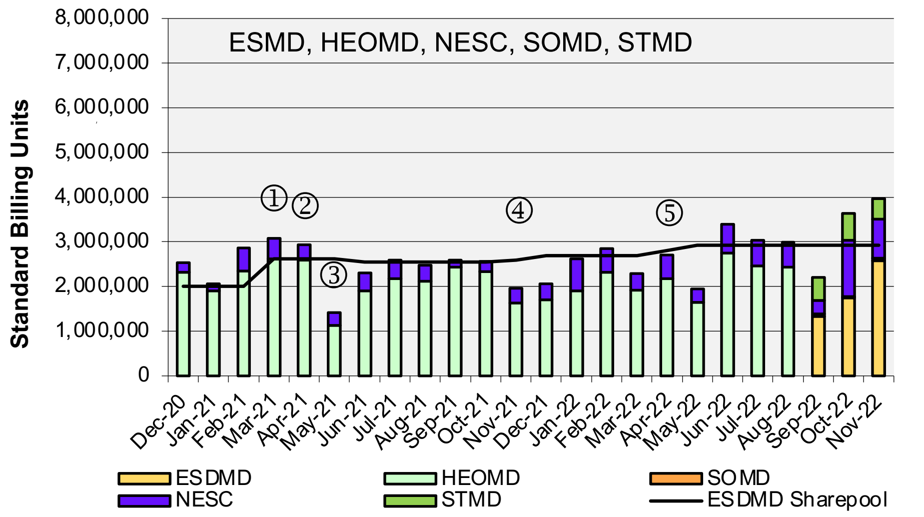






① 8 Rome Apollo racks introduced into Aitken

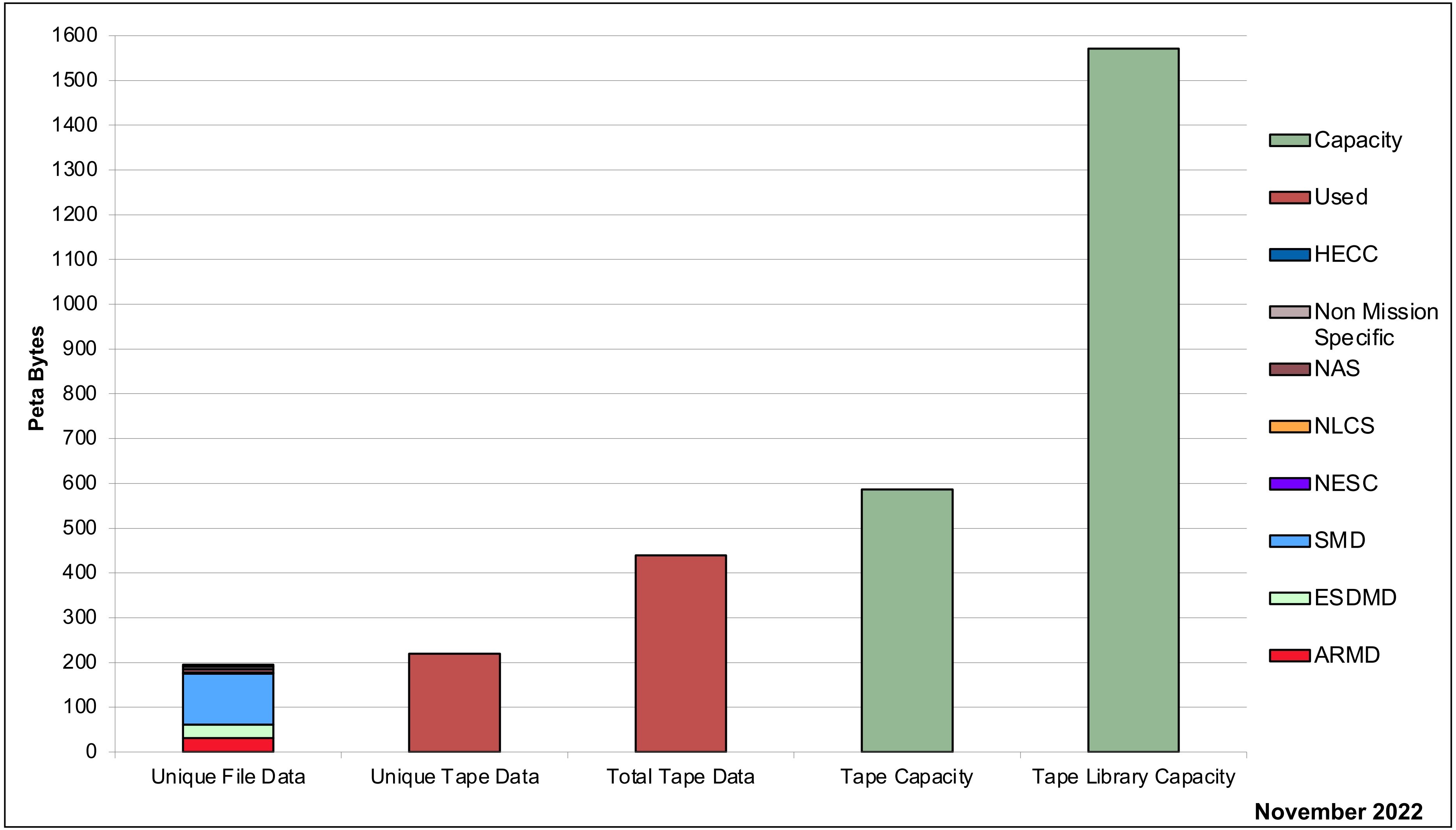
② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

⑤ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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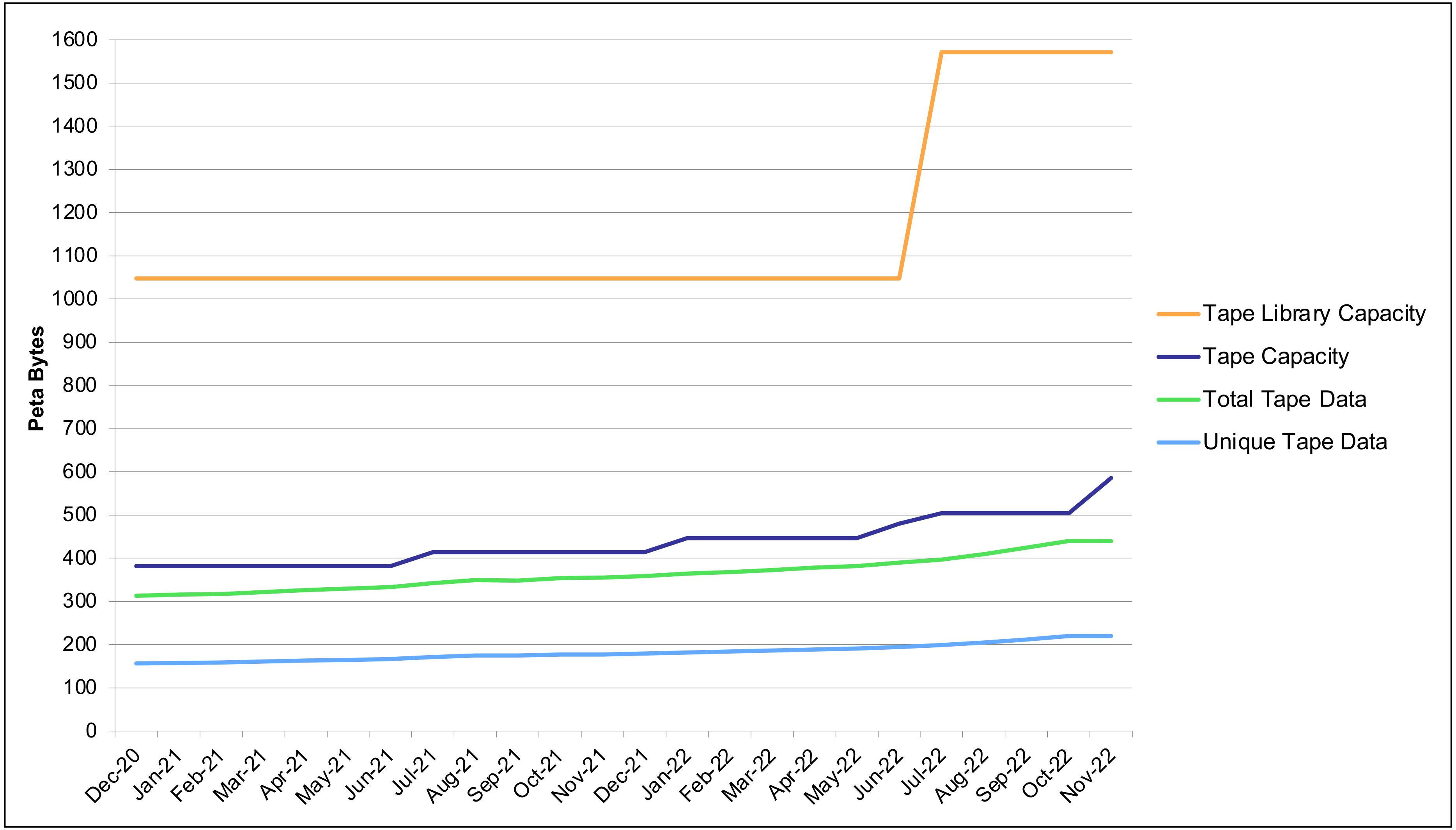
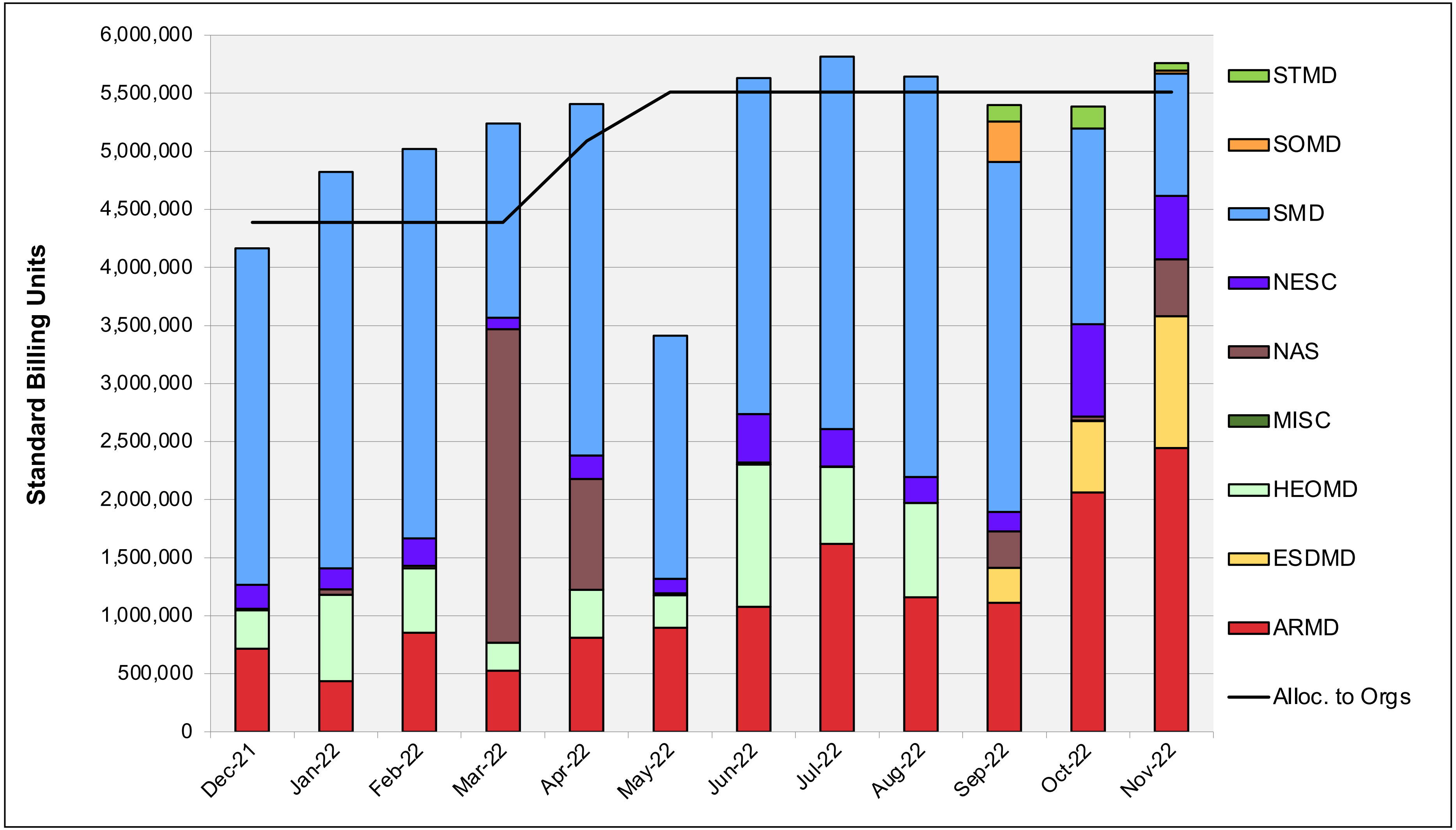
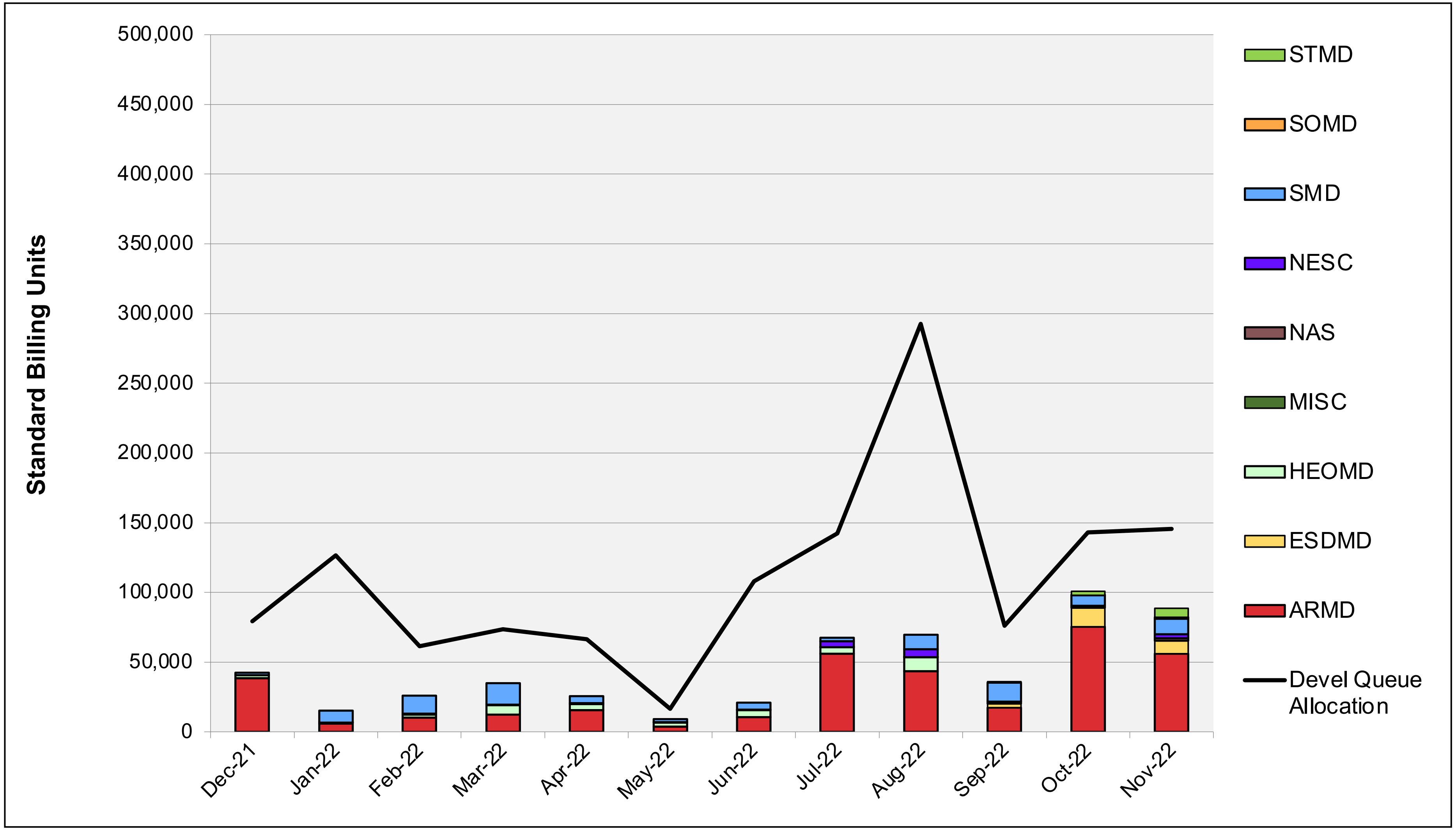


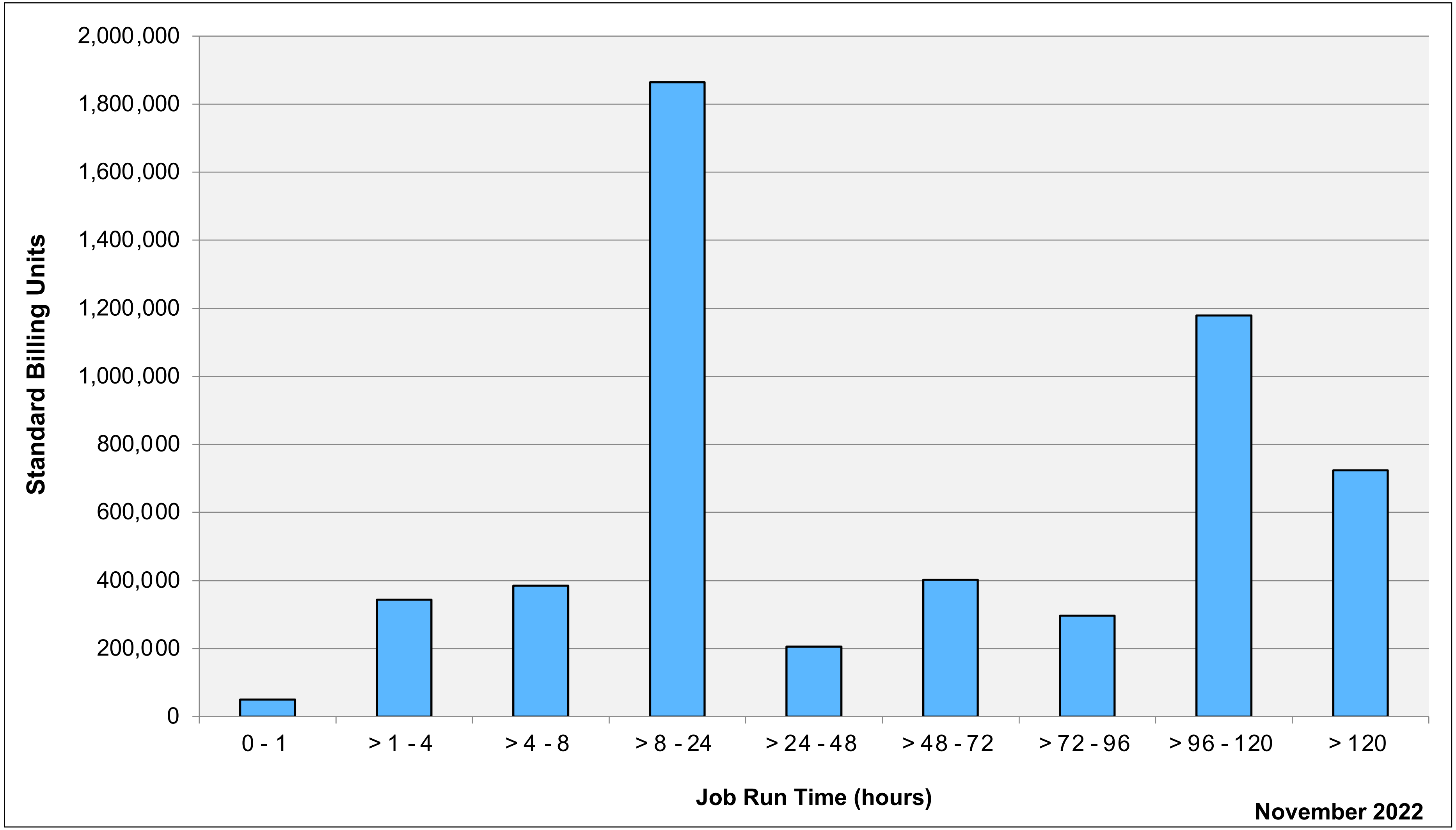
Aitken: SBUs Reported, Normalized to 30-Day Month



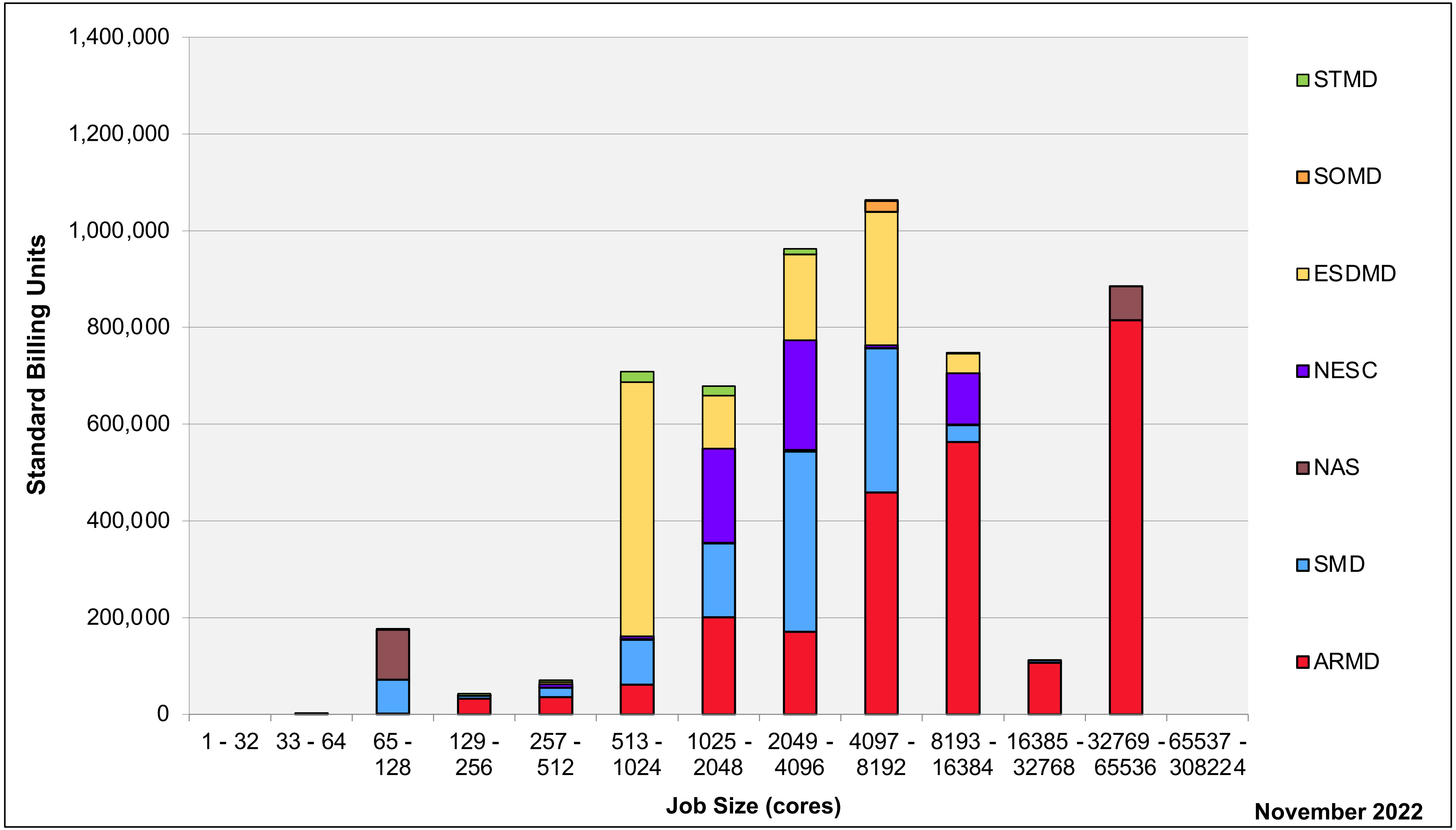
Aitken: Devel Queue Utilization



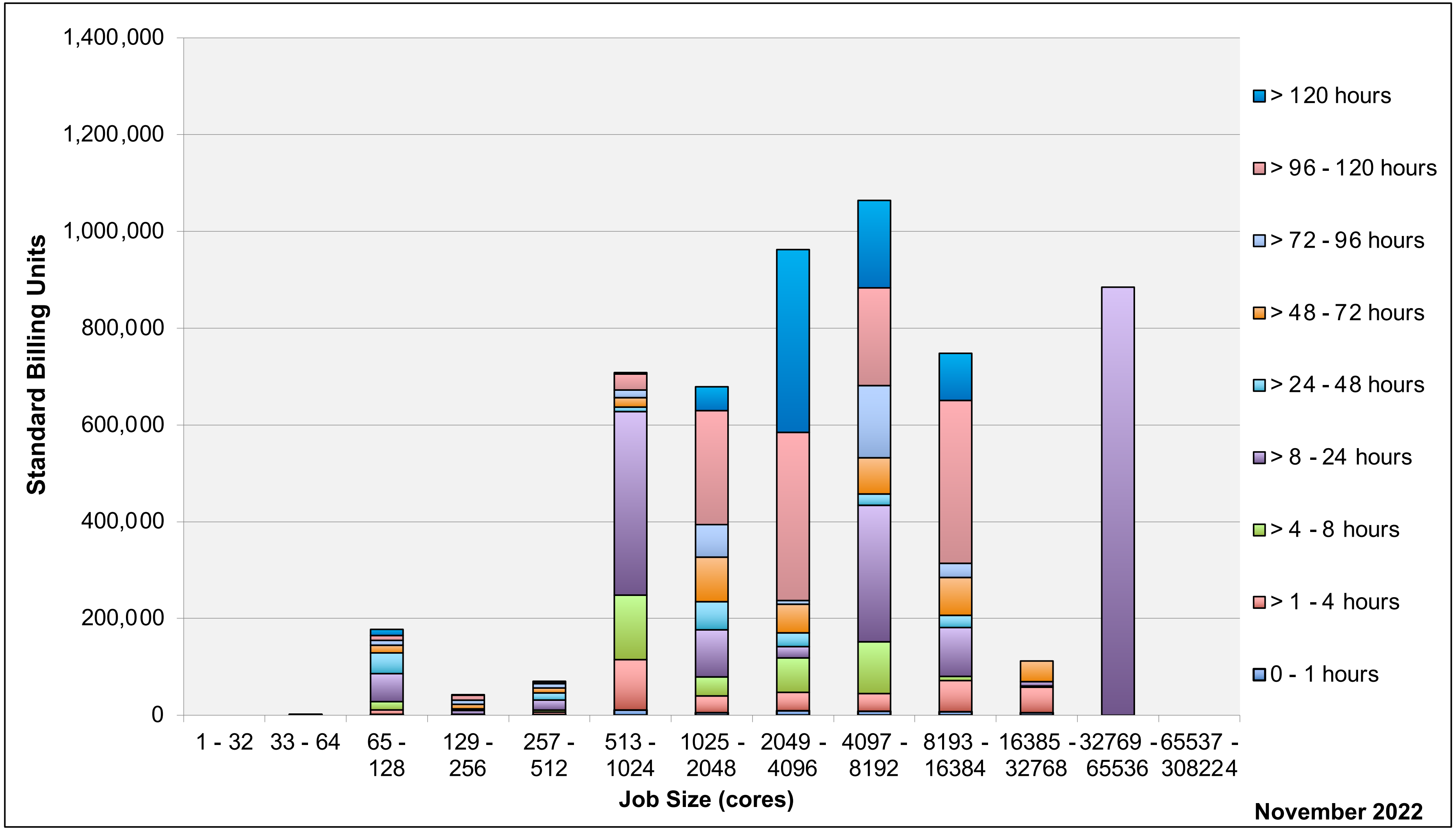
Aitken: Monthly Utilization by Job Length



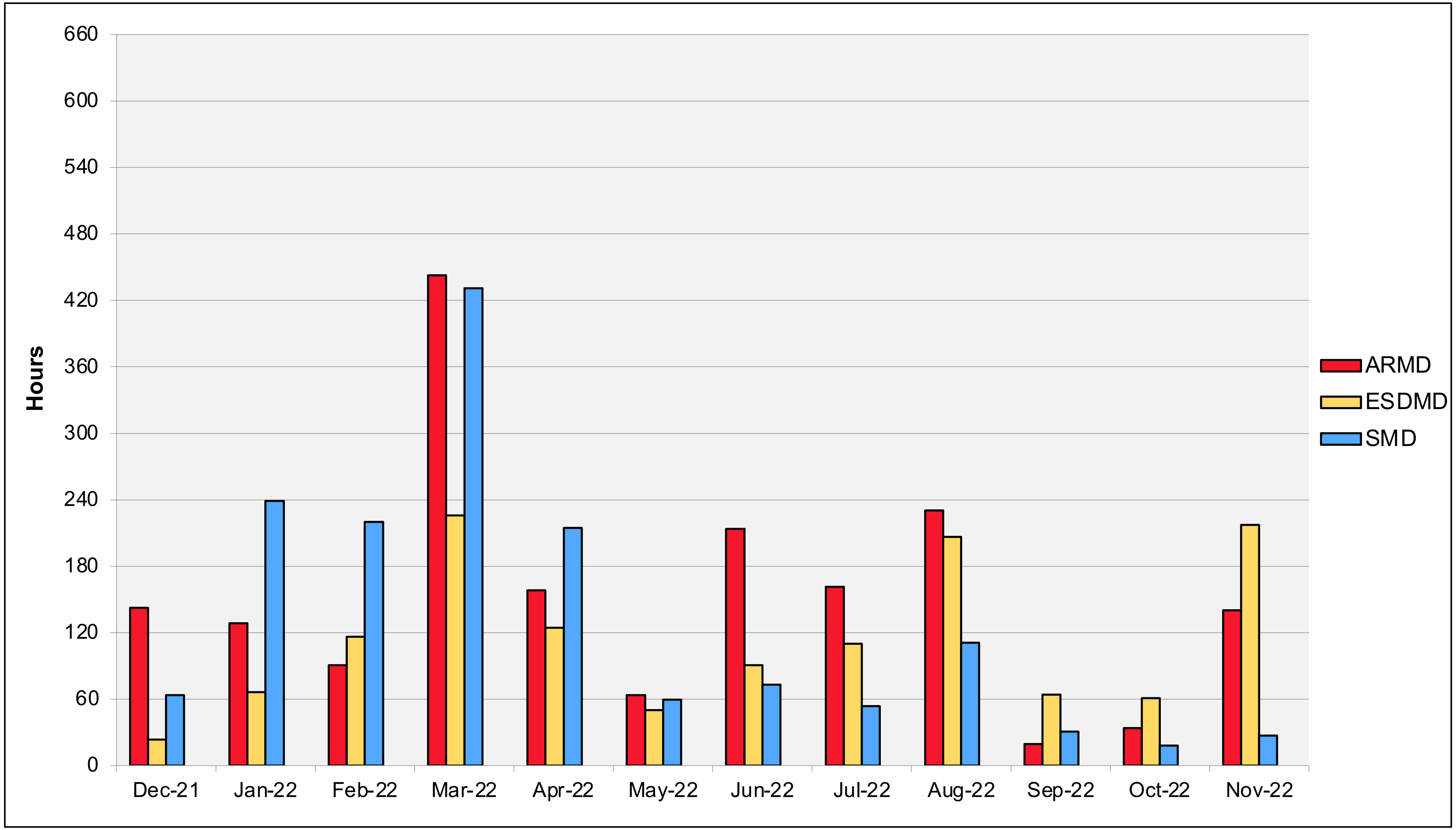
Aitken: Monthly Utilization by Job Size



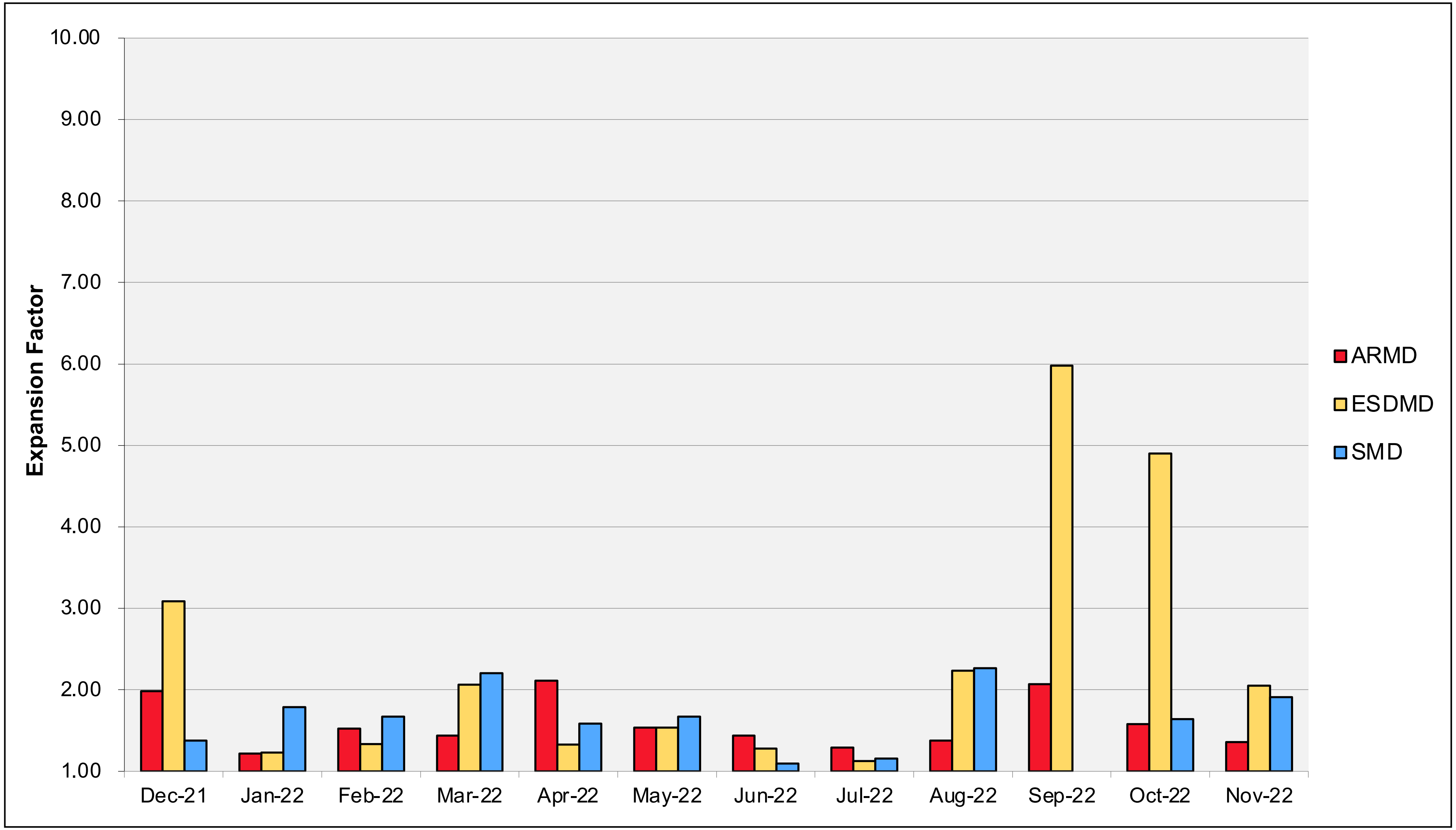
Aitken: Monthly Utilization by Size and Length



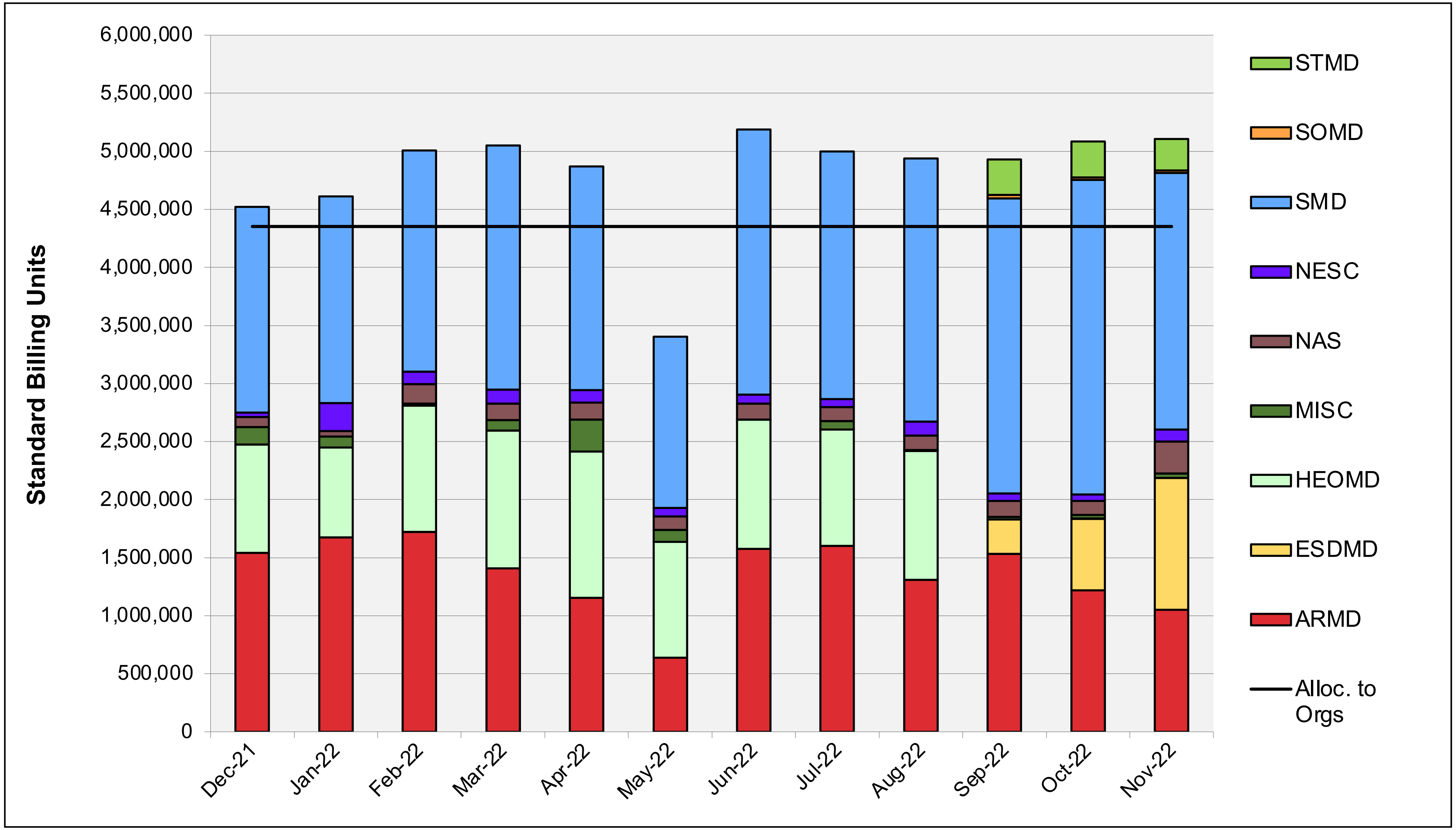
Aitken: Average Time to Clear All Jobs



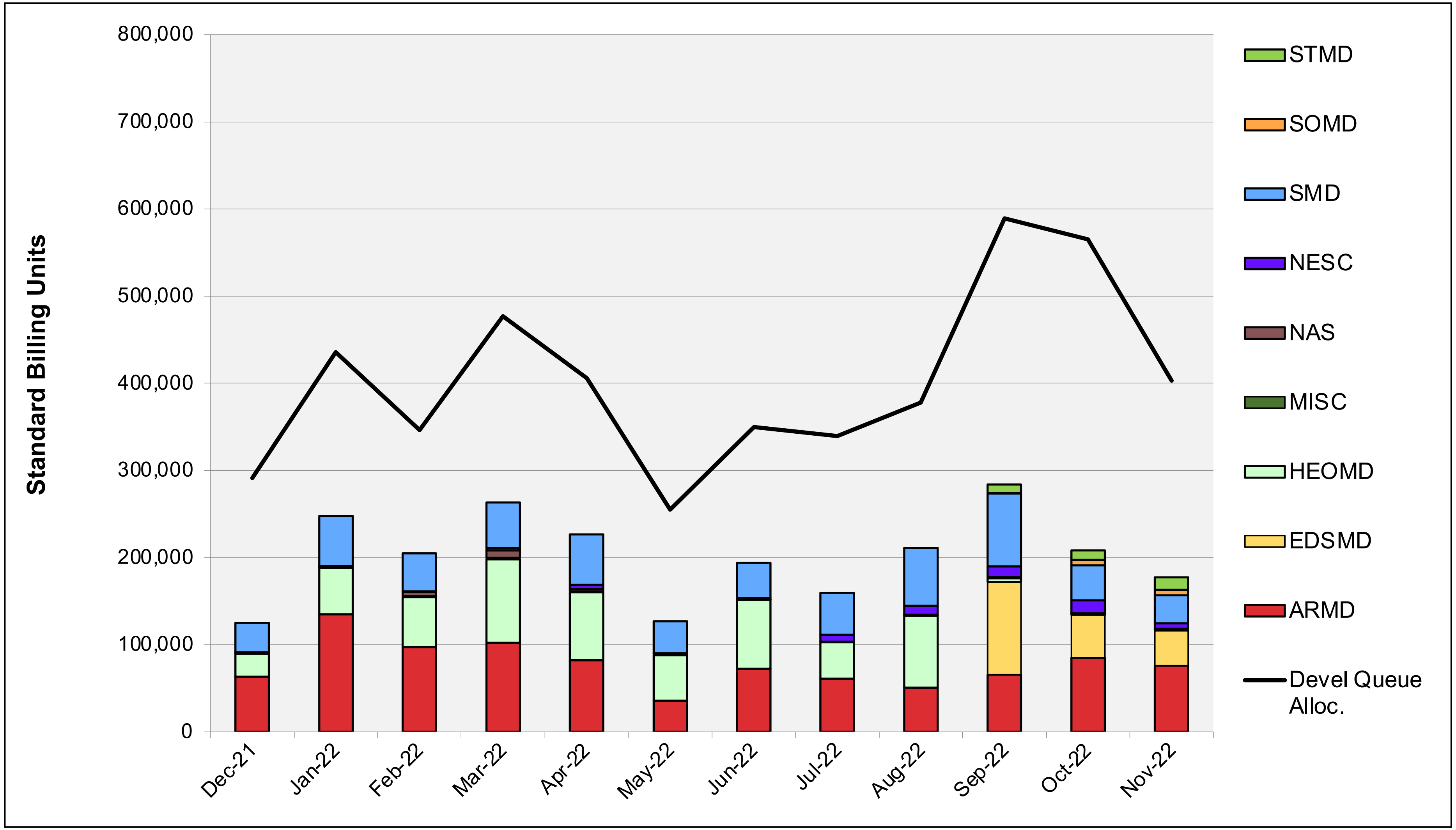
Aitken: Average Expansion Factor



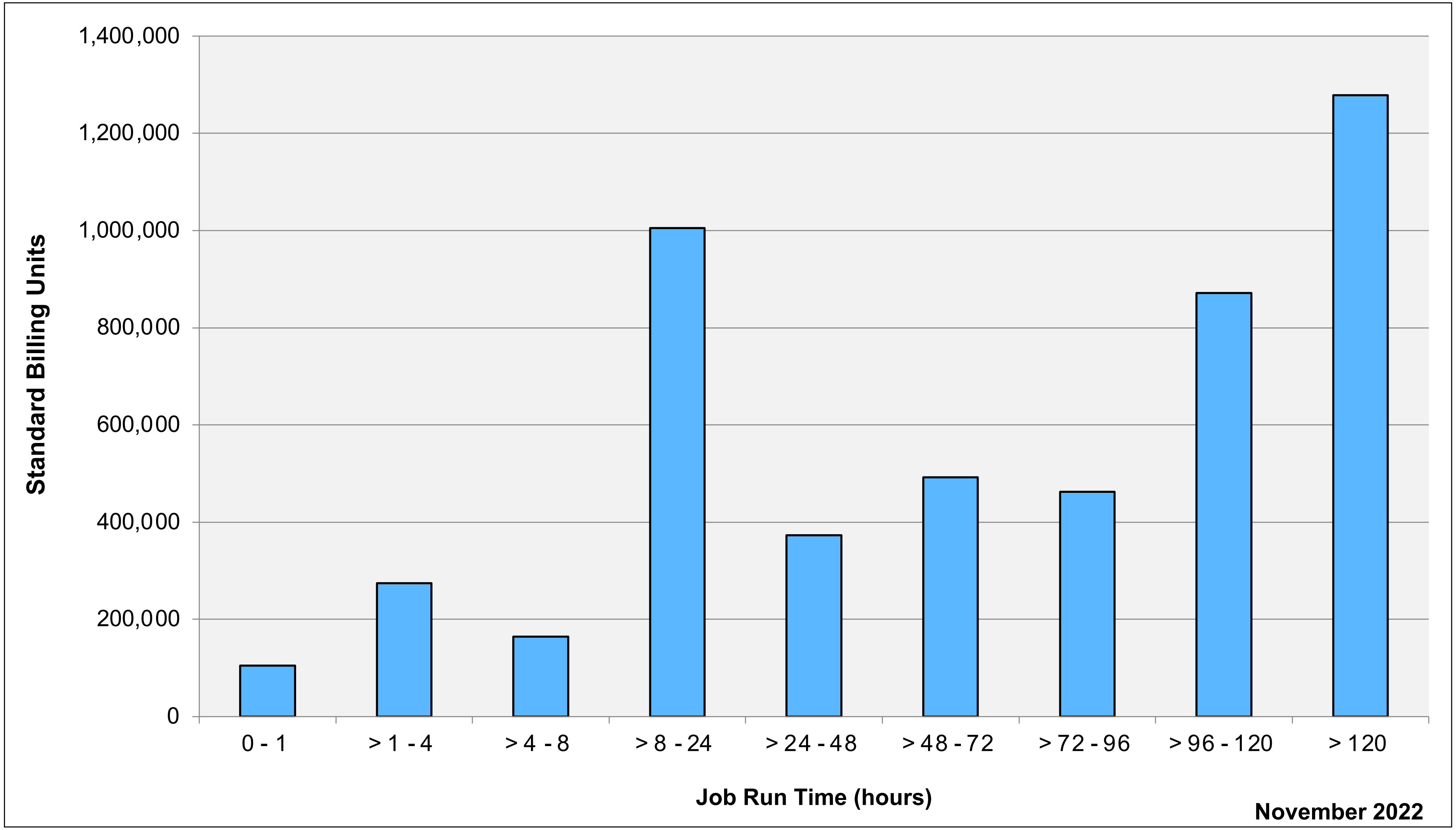
Pleiades: SBUs Reported, Normalized to 30-Day Month



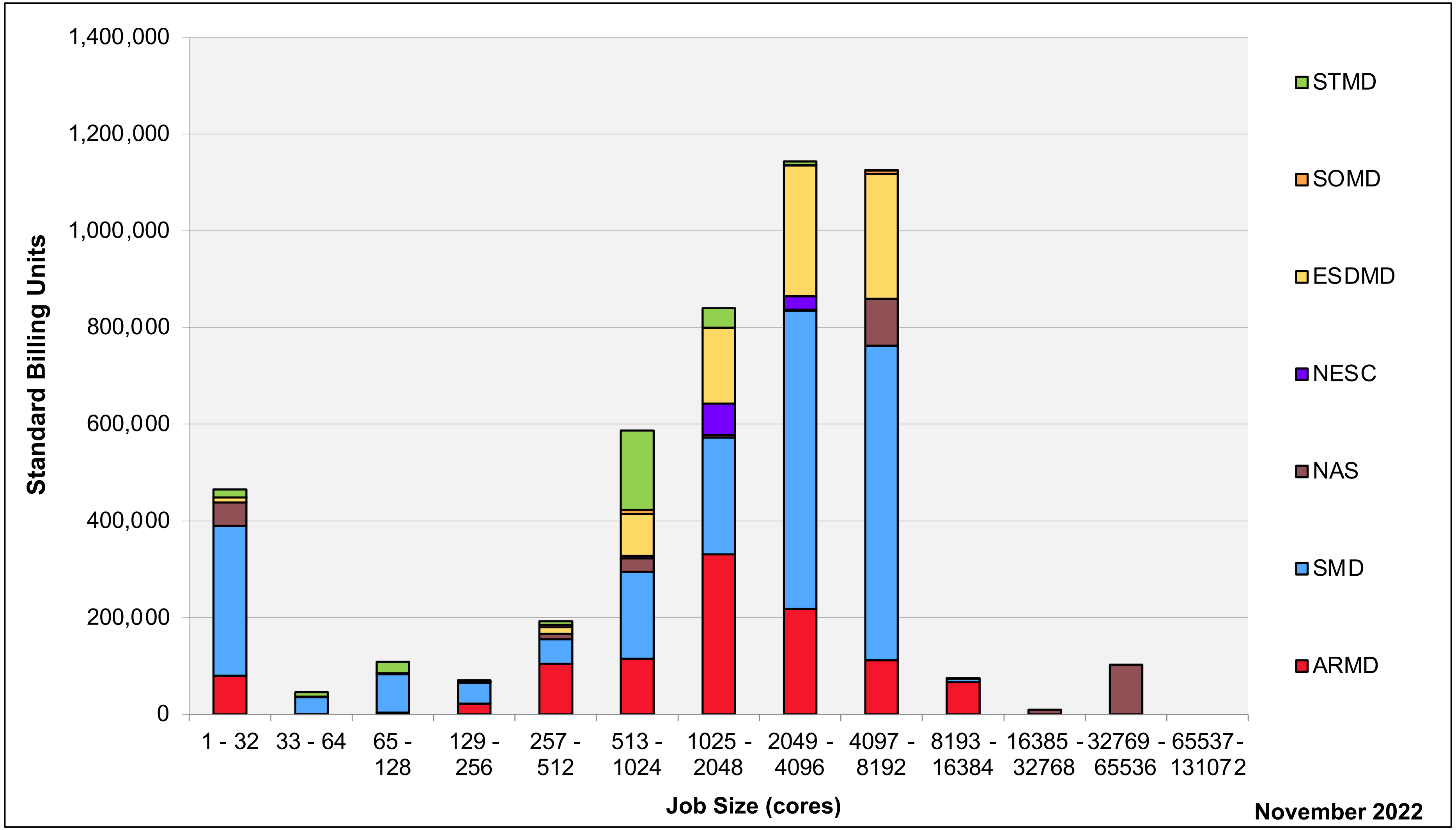
Pleiades: Devel Queue Utilization



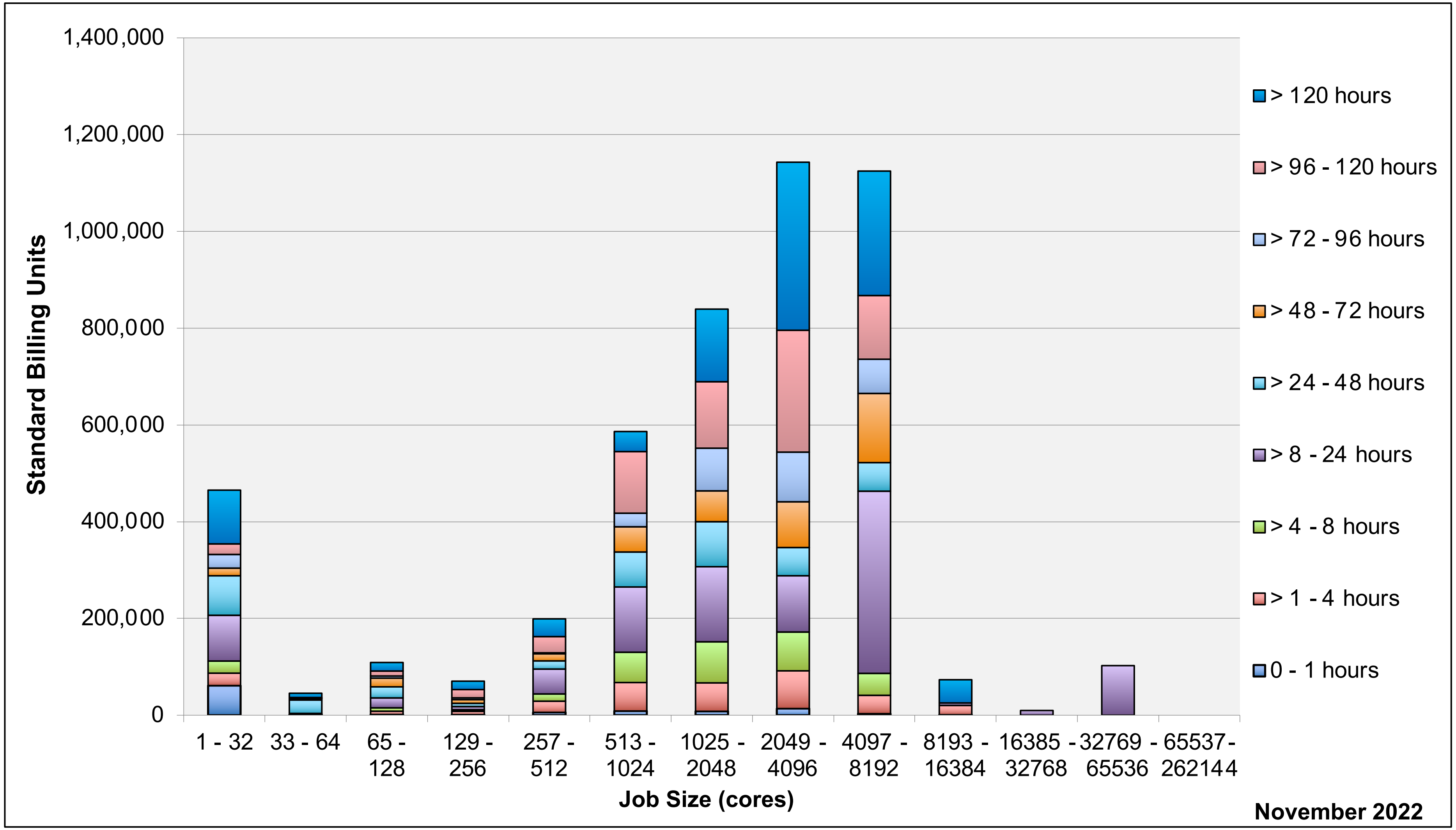
Pleiades: Monthly Utilization by Job Length



Pleiades: Monthly Utilization by Job Size



Pleiades: Monthly Utilization by Size and Length



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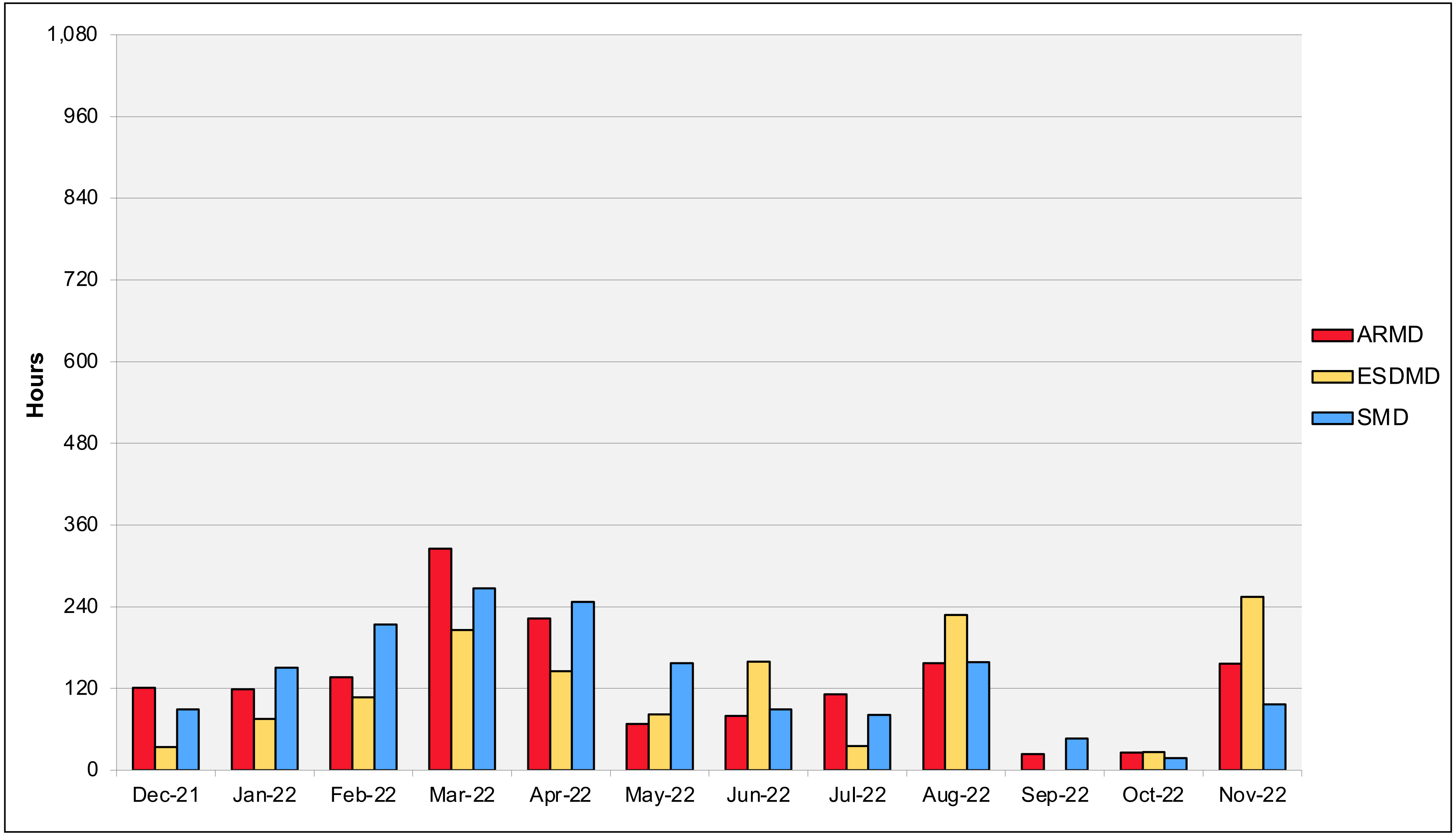
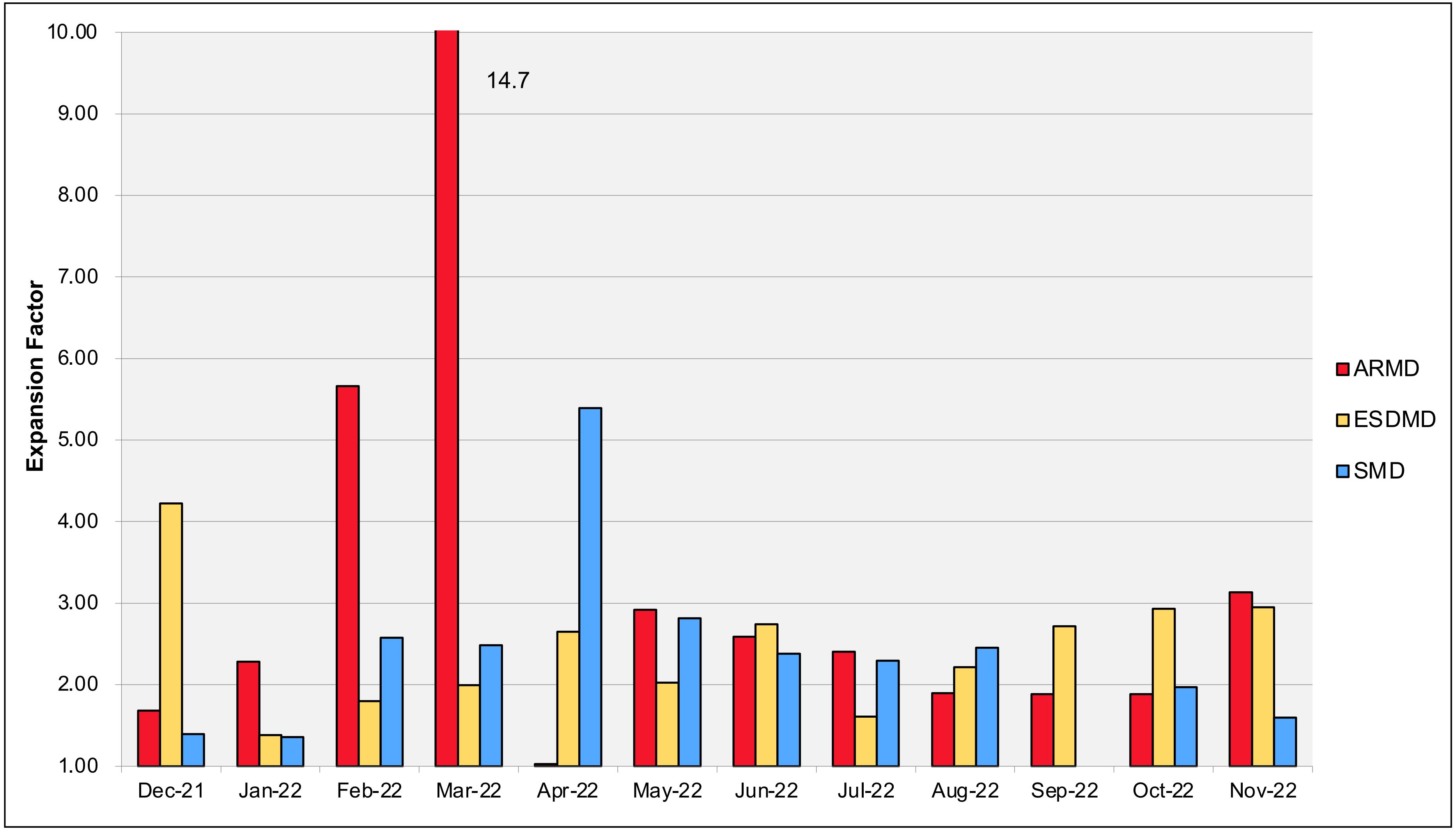
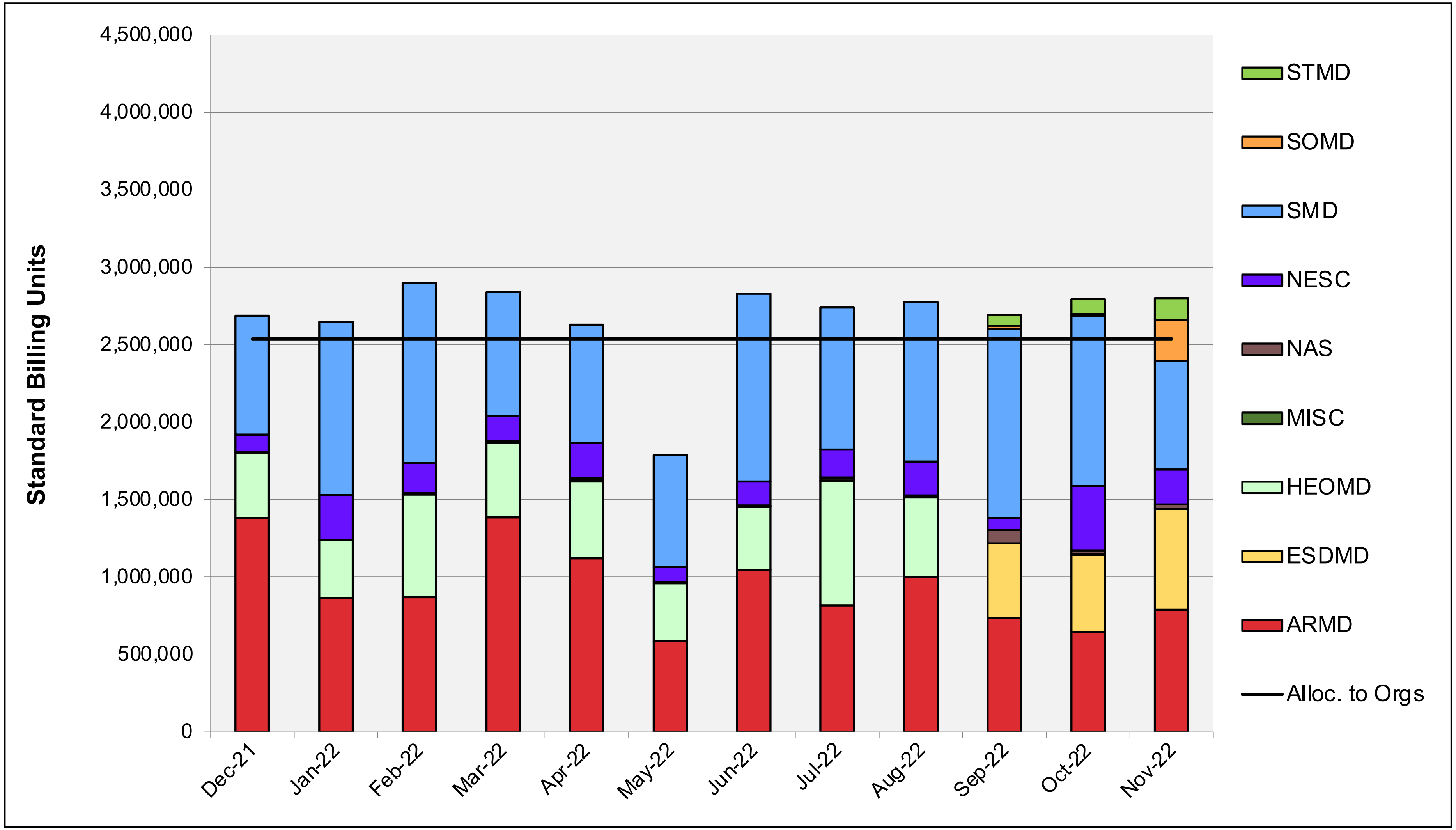


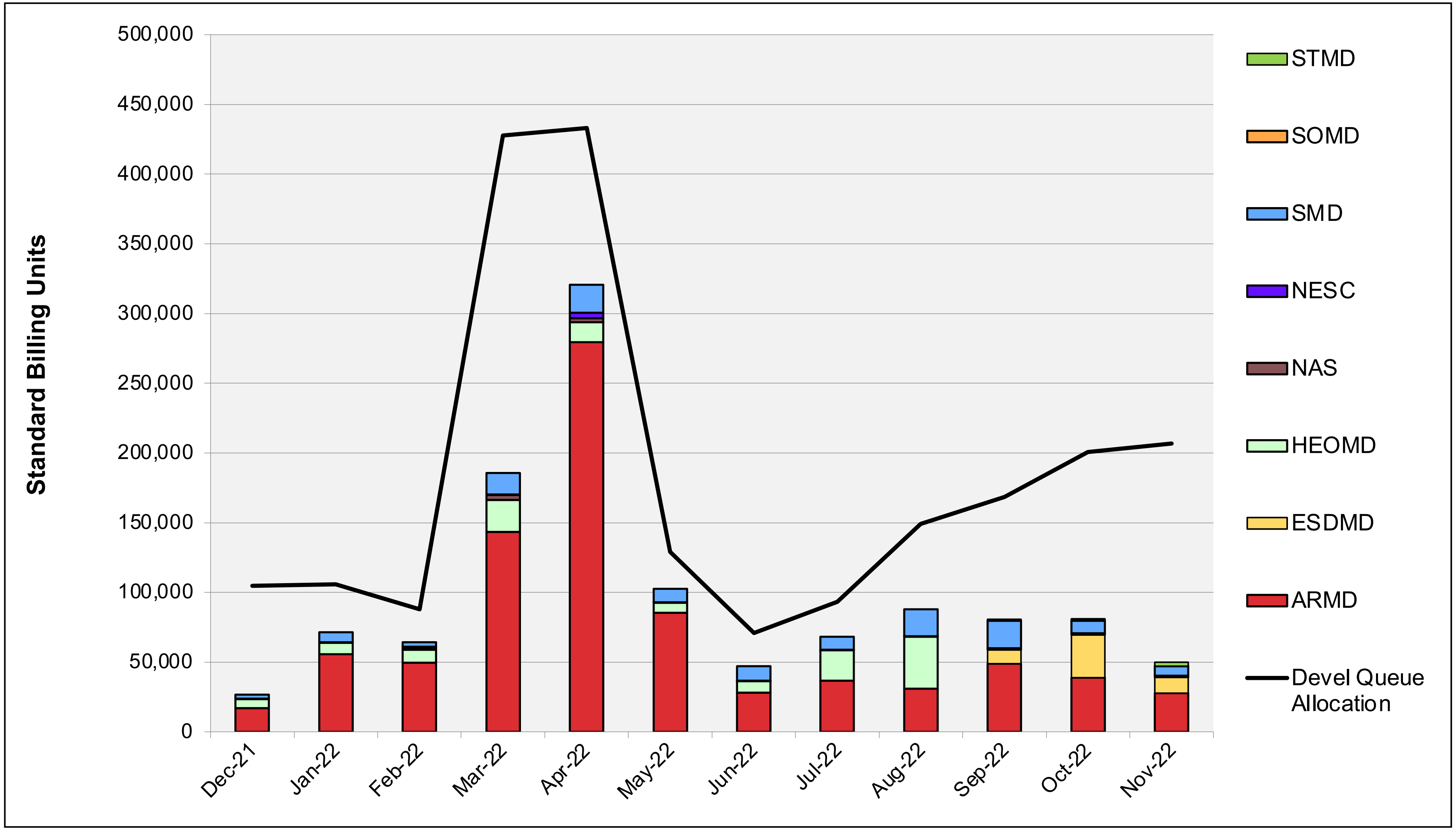
Pleiades: Average Expansion Factor



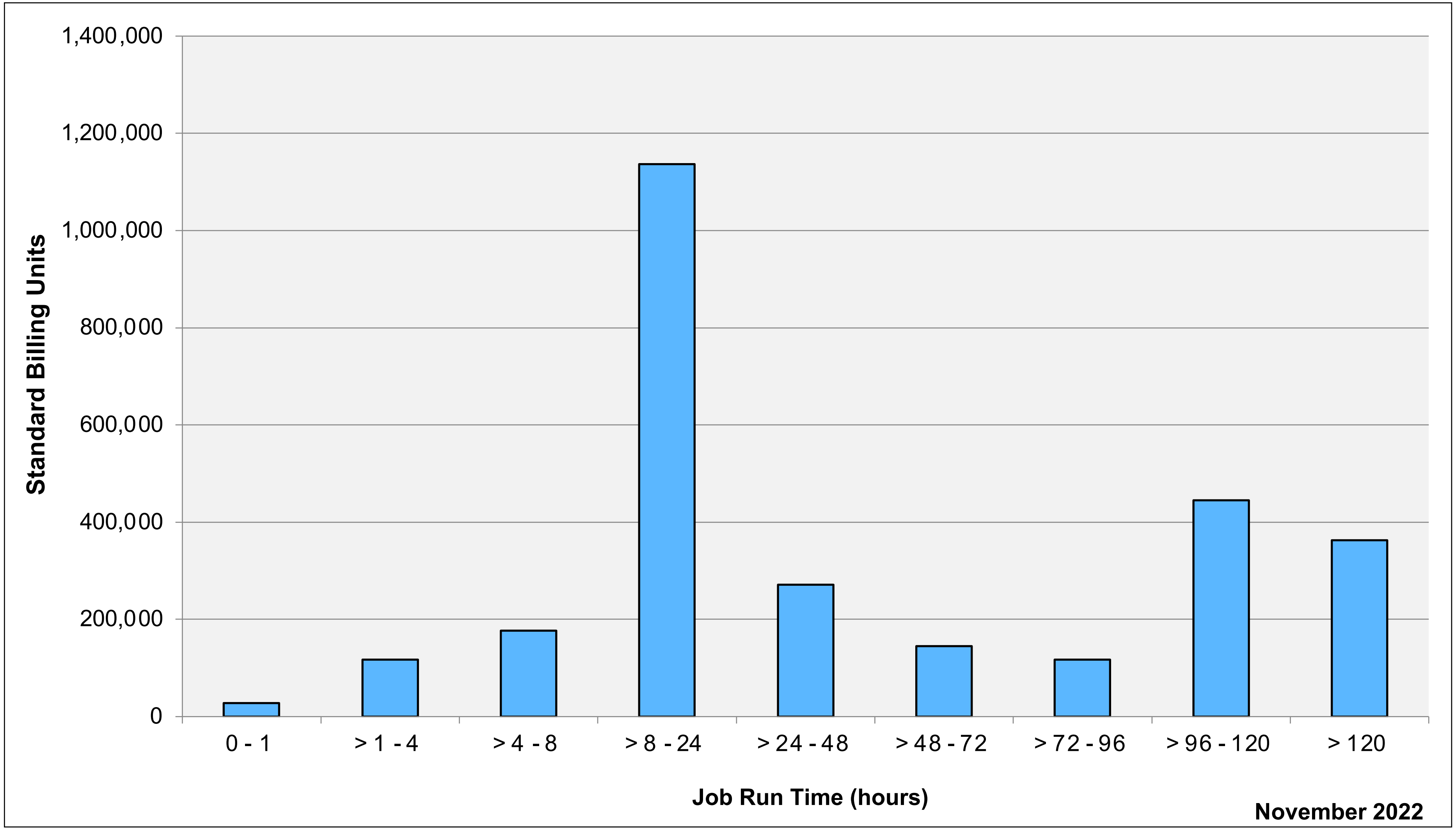
Electra: SBUs Reported, Normalized to 30-Day Month



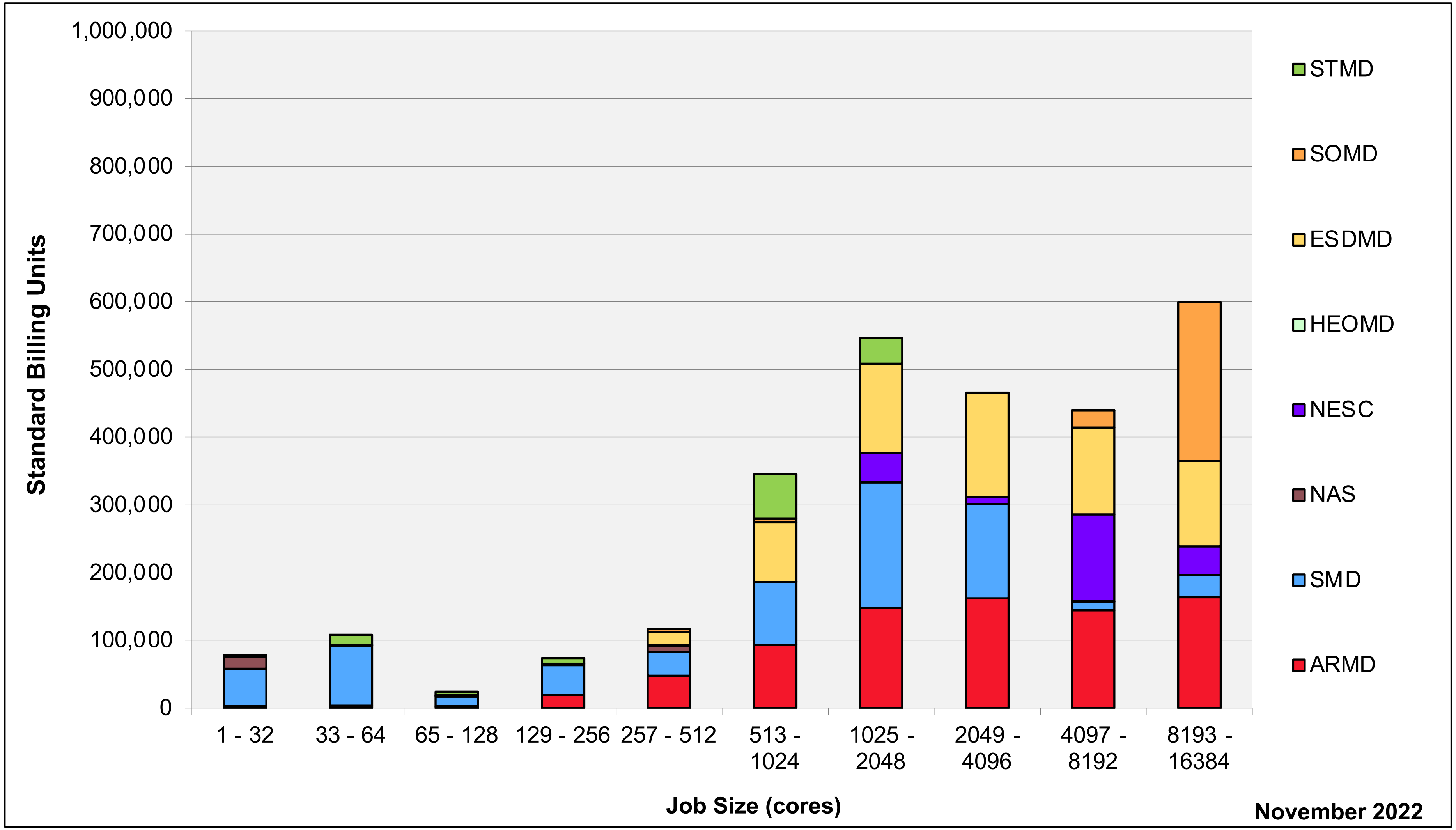
Electra: Devel Queue Utilization



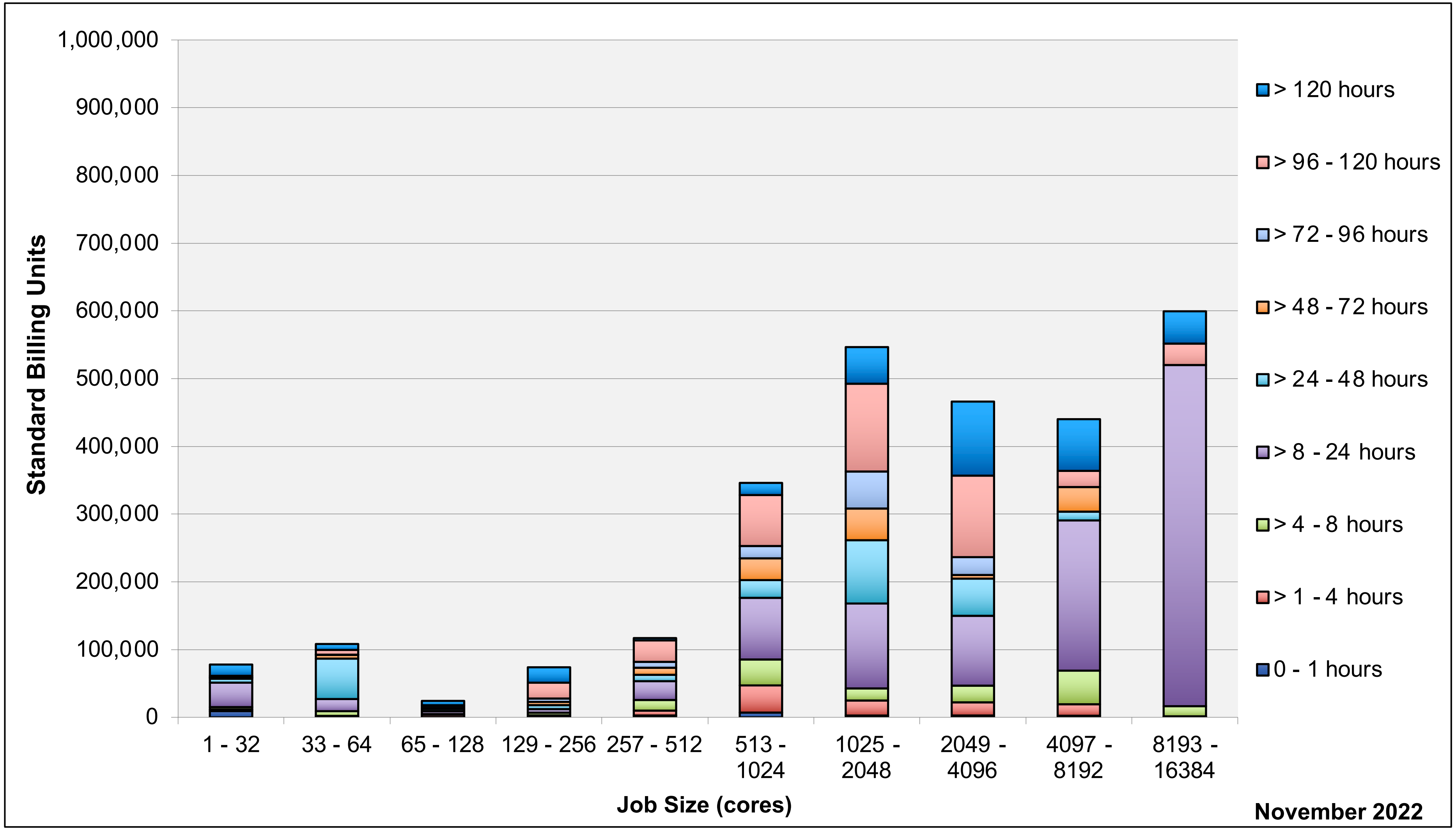
Electra: Monthly Utilization by Job Length



Electra: Monthly Utilization by Job Size



Electra: Monthly Utilization by Size and Length



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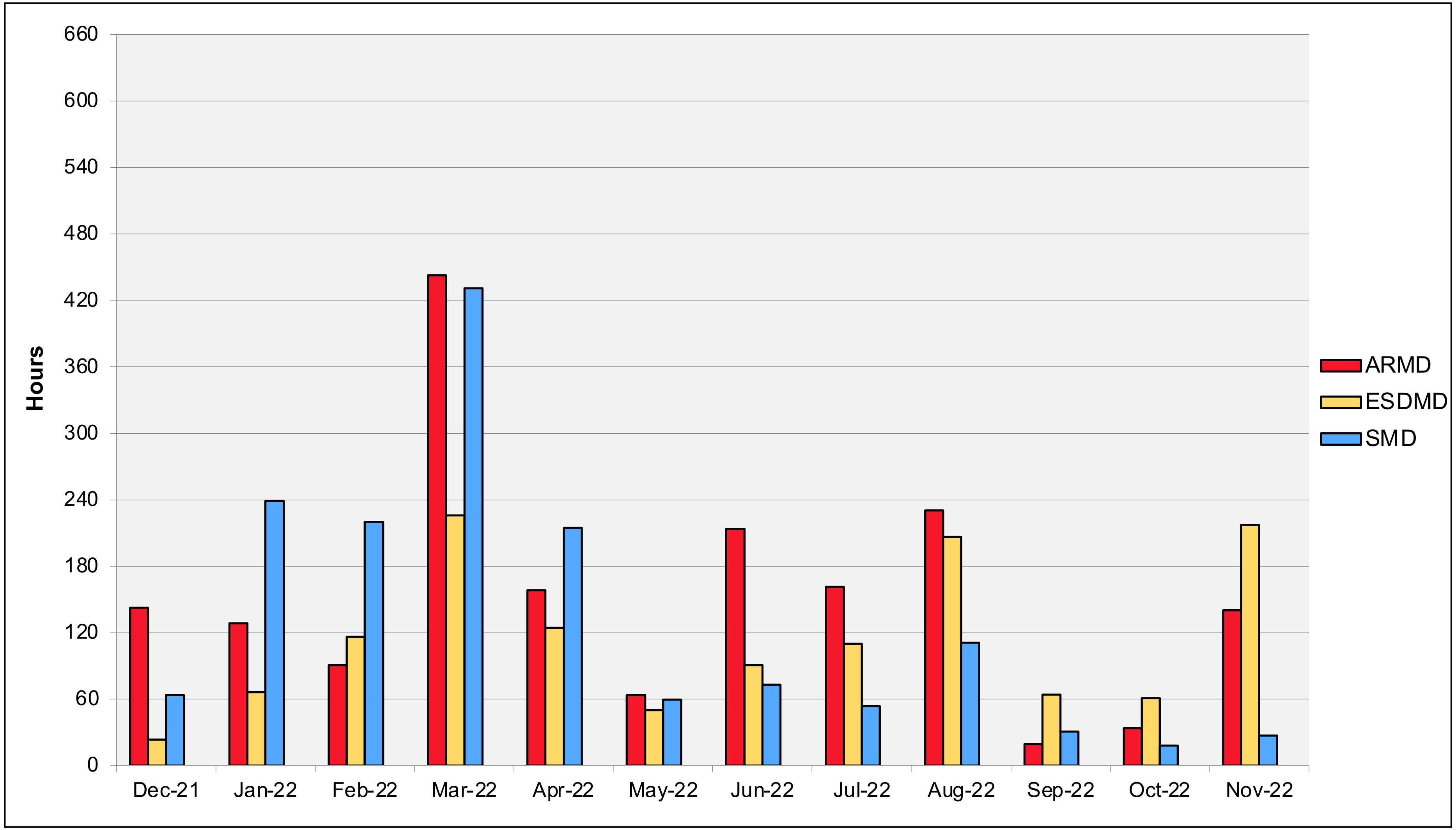

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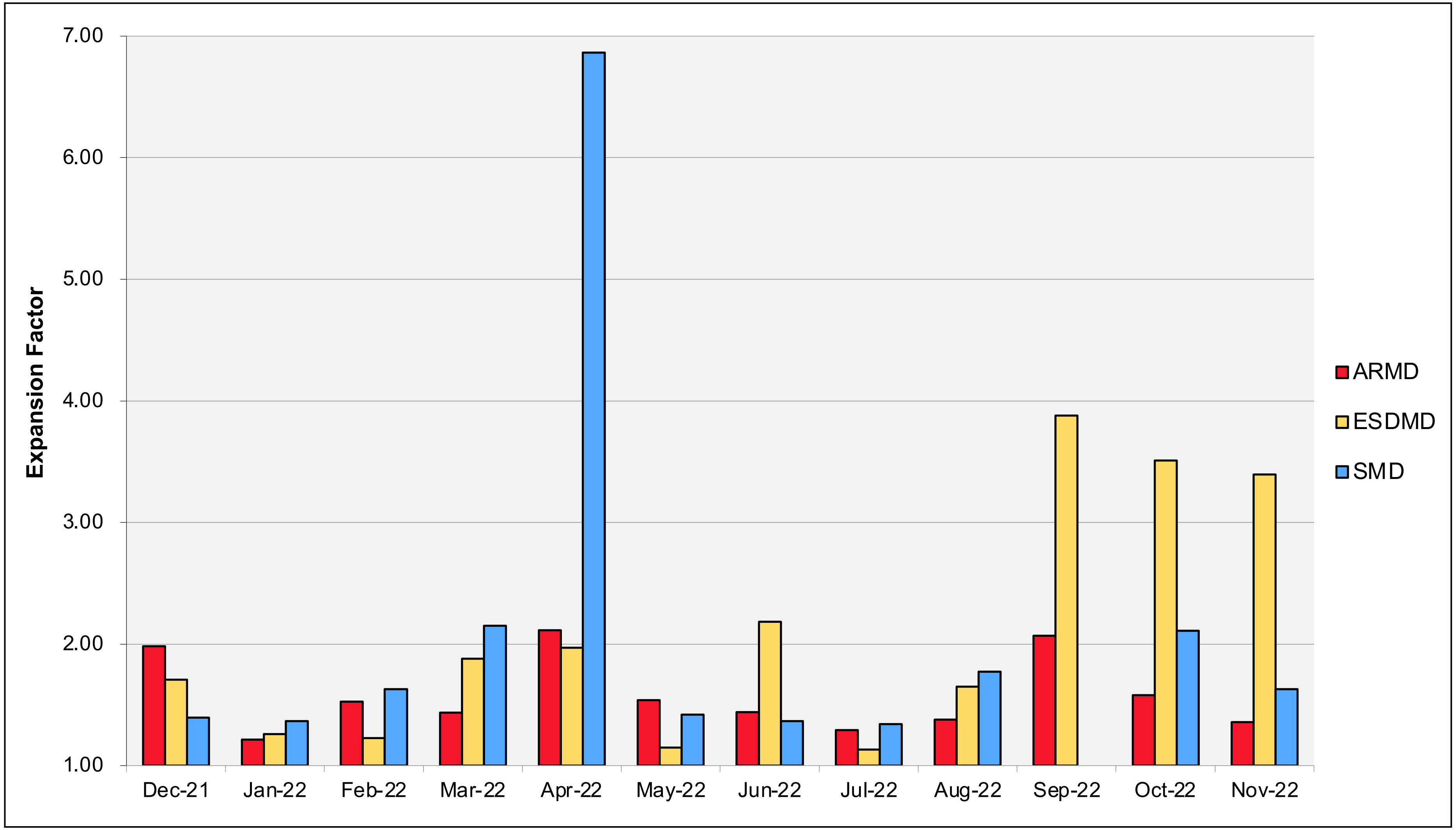
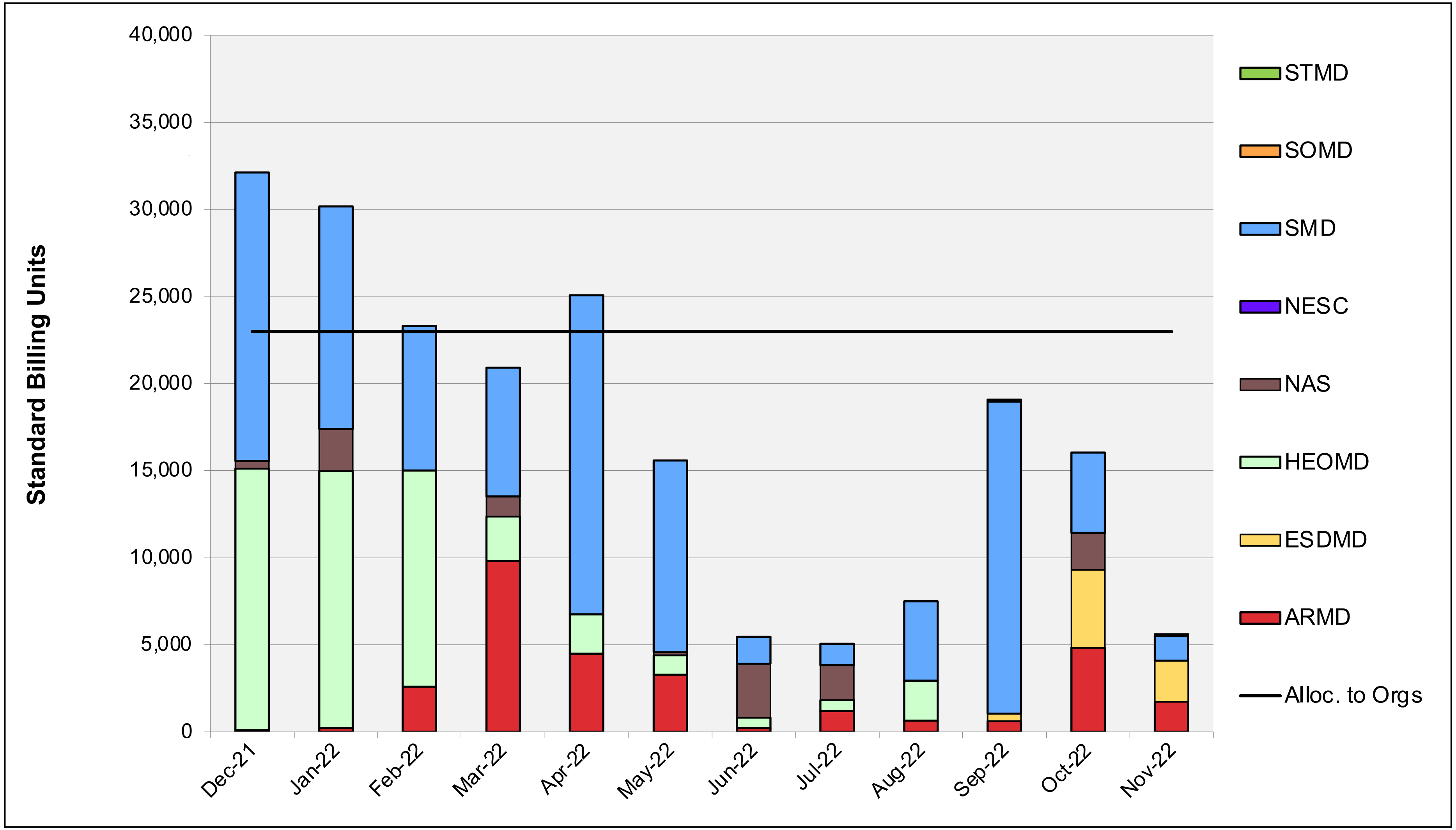
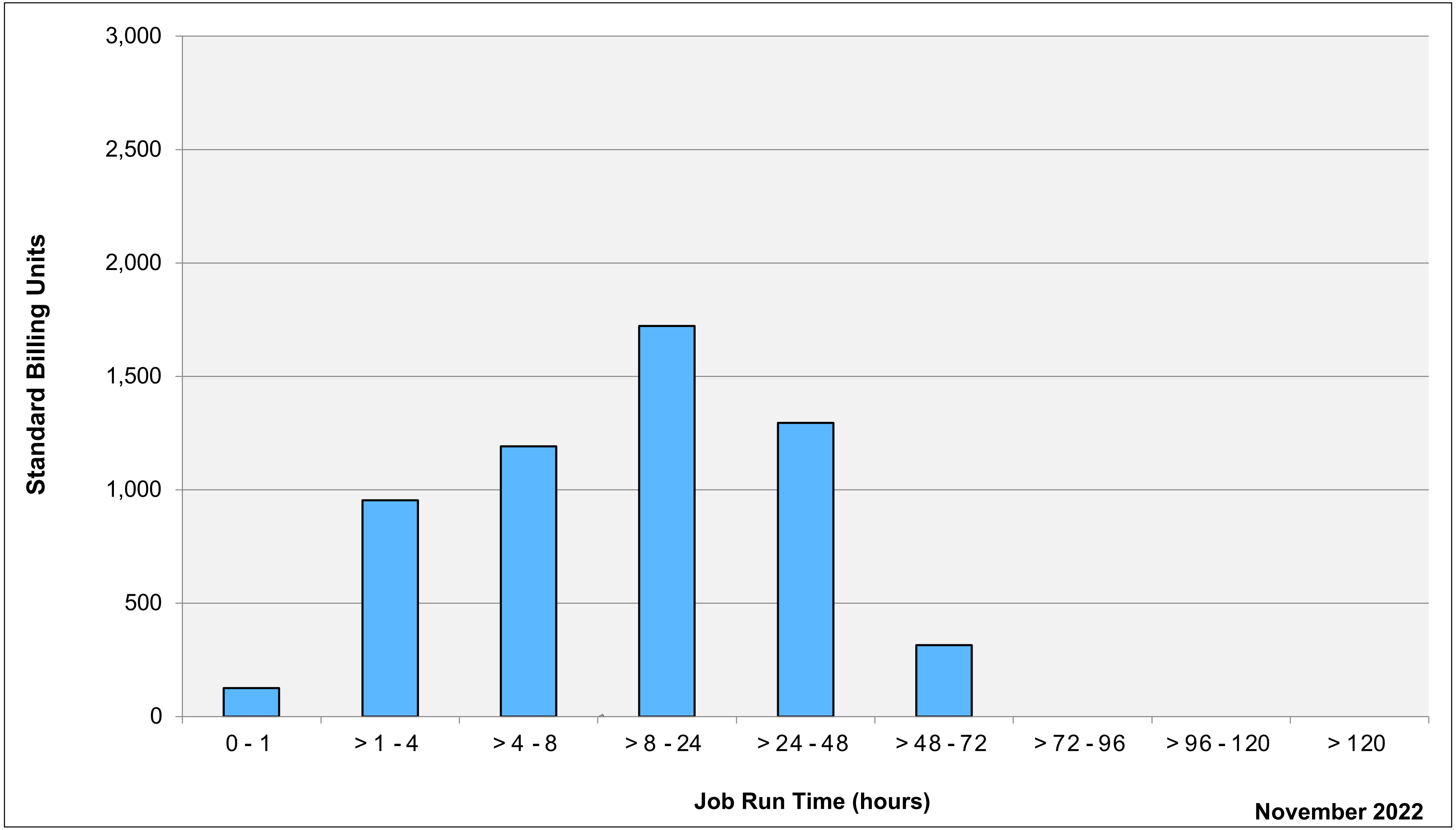


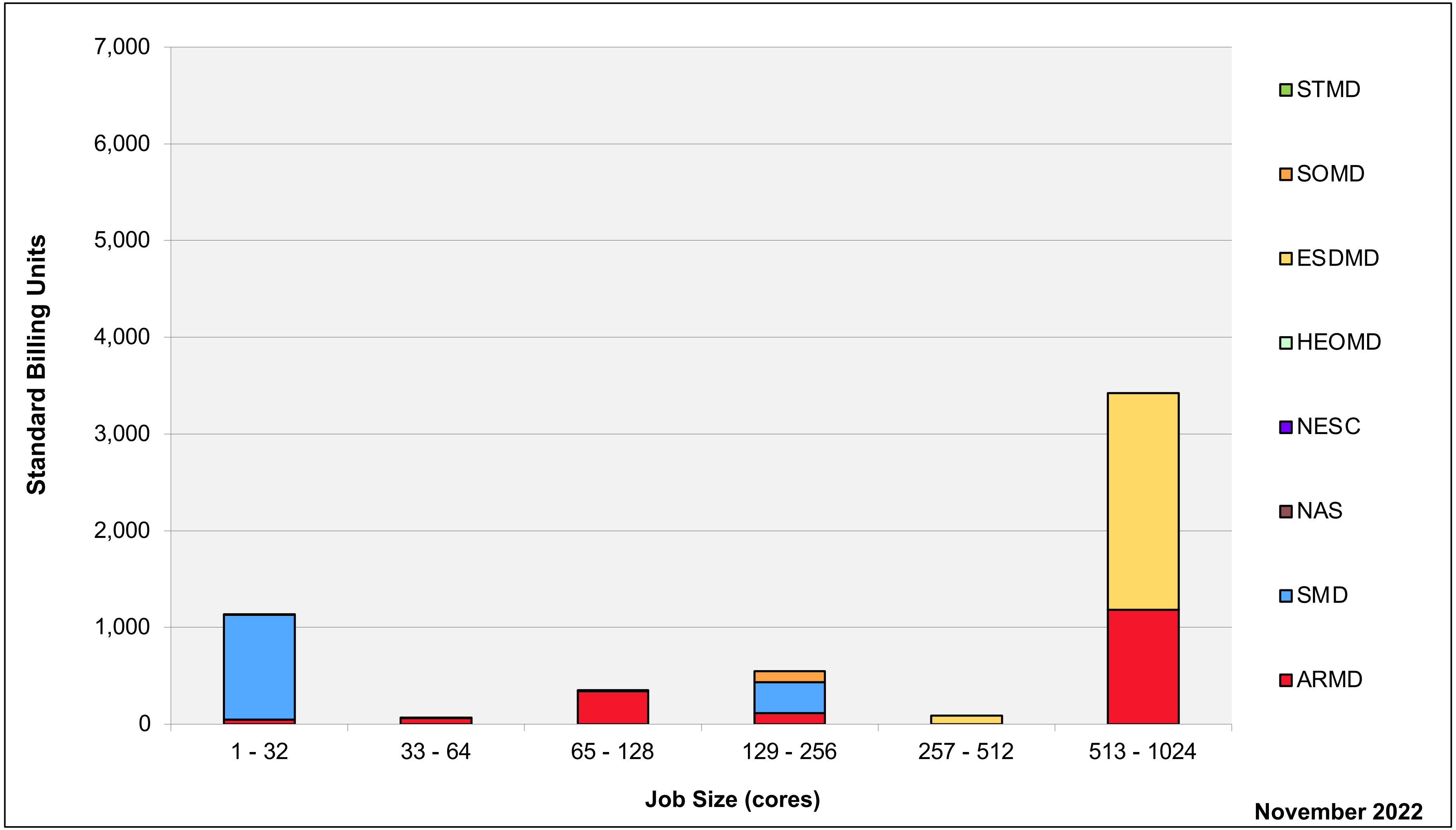
Endeavour: SBUs Reported, Normalized to 30-Day Month



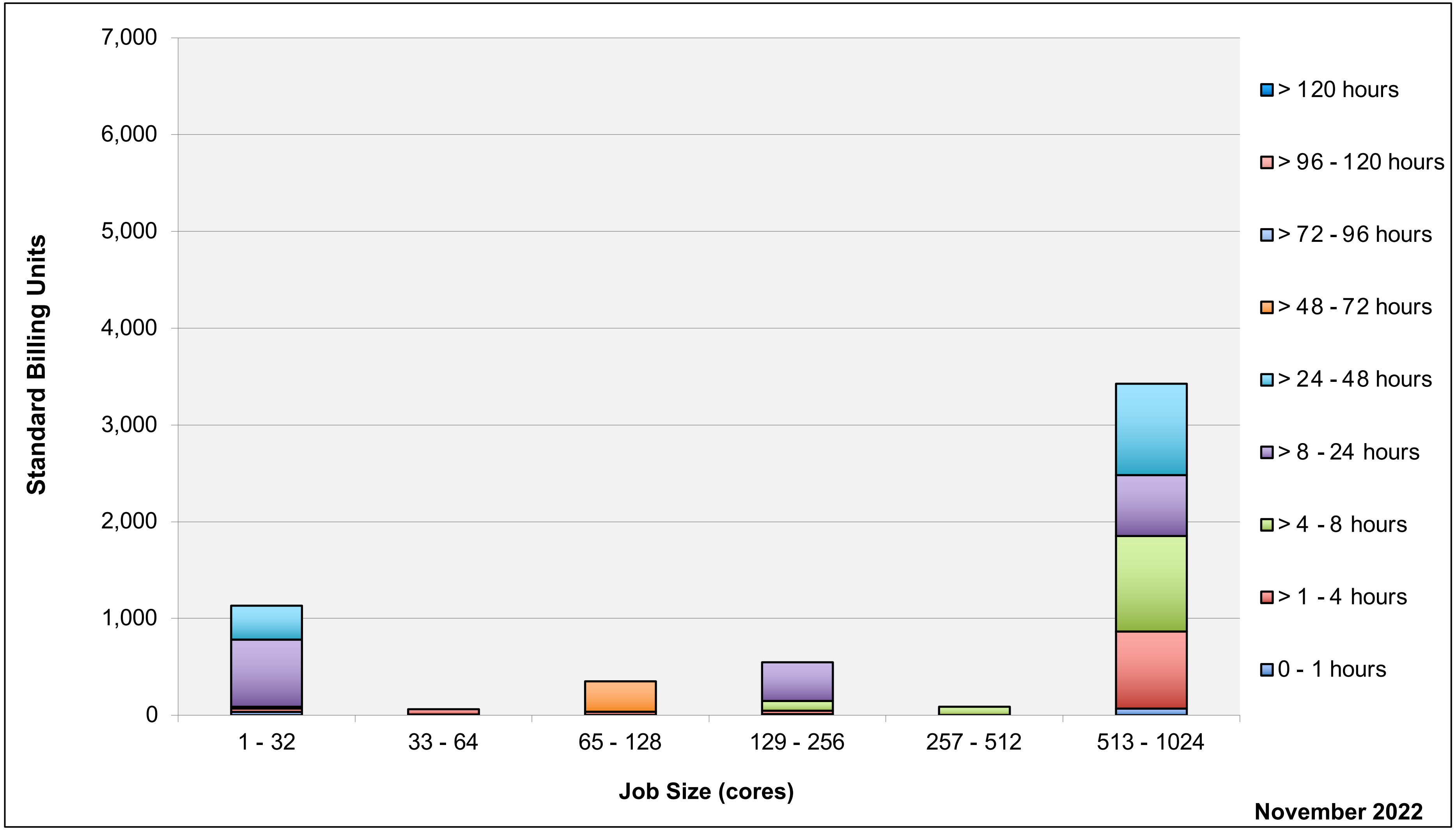
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor